STIC Search Report
Biotech-Chem Library

STIC Database Tracking Number: 133273

TO:	From:
Ben Sackey Location: rem/5b31/5c18 Art Unit: 1626 Wednesday, September 22, 2004 Case Serial Number: 10/786992	Noble Jarrell Location: Biotech-Chem Library Rem 1B71 Phone: 272-2556 Noble.jarrell@uspto.gov

Search Notes

Blank Sheet

Noble.

Access DB# 133273

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: BEN SACKEY Examiner #: 73489 Date: 9/21/04
Art Unit: 1626 Phone Number 30[illegible]2-0704 Serial Number: 10/786,992
Mail Box and Bldg/Room Location: REM 5B31 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

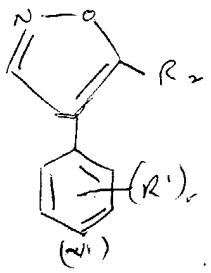
Title of Invention: Convergent Synthesis of alpha-aryl-beta-ketonitriles

Inventors (please provide full names): Jincheng Zhou et al.

Earliest Priority Filing Date: 4/3/98

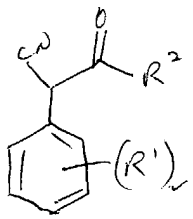
For Sequence Searches Only *Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

Compds & claims 10 and 11 respectively



(II)

claim 10 substituents are as defined in the claim.



(I)

claim 11 substituents are as defined in the claim.

Thanks

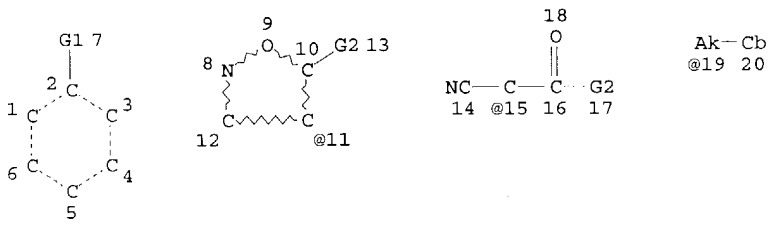
****

STAFF USE ONLY	Type of Search	Vendors and cost where applicable
Searcher: Noble	NA Sequence (#)	STN 685
Searcher Phone #:	AA Sequence (#)	Dialog
Searcher Location:	Structure (#) 1	Questel/Orbit
Date Searcher Picked Up:	Bibliographic	Dr.Link
Date Completed: 9/22/04	Litigation	Lexis/Nexis
Searcher Prep & Review Time: 30	Fulltext	Sequence Systems
Clerical Prep Time:	Patent Family	WWW/Internet
Online Time: 30	Other	Other (specify)

PTO-1590 (8-01)

Blank Sheet

```
=> b reg
FILE 'REGISTRY' ENTERED AT 14:39:57 ON 22 SEP 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   21 SEP 2004  HIGHEST RN 749178-43-6
DICTIONARY FILE UPDATES:  21 SEP 2004  HIGHEST RN 749178-43-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> d que stat l9
L7                STR
```




```
VAR G1=11/15
VAR G2=H/AK/CB/19/21/23
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC   1   8
NUMBER OF NODES IS  24

STEREO ATTRIBUTES: NONE
L9          4442 SEA FILE=REGISTRY SSS FUL L7

100.0% PROCESSED   9936 ITERATIONS                      4442 ANSWERS
SEARCH TIME: 00.00.01


=> d his

     FILE 'HCAPLUS' ENTERED AT 13:07:05 ON 22 SEP 2004
L1             1 US20040171829/PN

     FILE 'REGISTRY' ENTERED AT 13:07:11 ON 22 SEP 2004

     FILE 'HCAPLUS' ENTERED AT 13:07:14 ON 22 SEP 2004
L2               TRA L1 1- RN :       13 TERMS

     FILE 'REGISTRY' ENTERED AT 13:07:14 ON 22 SEP 2004
L3            13 SEA L2

     FILE 'WPIX' ENTERED AT 13:07:16 ON 22 SEP 2004
L4             1 US20040171829/PN
```

```
     FILE 'REGISTRY' ENTERED AT 13:18:34 ON 22 SEP 2004
L5                STR
L6             23 L5
L7                STR L5
L8             50 L7
L9           4442 L7 FULL
                  SAVE TEMP SAC992F0/A L9

     FILE 'HCAPLUS' ENTERED AT 13:33:19 ON 22 SEP 2004
L10          1698 L9

     FILE 'HCAOLD' ENTERED AT 13:33:27 ON 22 SEP 2004
L11           154 L9
                  SEL AN
                  EDIT E1-E154 /AN /OREF

     FILE 'HCAPLUS' ENTERED AT 13:34:14 ON 22 SEP 2004
L12           258 E1-154
L13          1806 L10 OR L12
                  E ZHOU J/AU
L14          1042 E3-31,E105
                  E ZHOU JIACHENG/AU
L15            28 E3
                  E OH L/AU
L16            10 E16-17
                  E MA P/AU
L17            97 E3-14
                  E MA PHILIP/AU
L18            39 E3-5
L19         56052 (DUPONT OR DU (1A) PONT)/CS,PA
L20             2 L13 AND L14-18
L21            10 L13 AND L19
L22             9 L21 NOT L20
L23          1804 L13 NOT L20
L24          1256 L23 AND (PY<=1998 OR AY<=1998 OR PRY<=1998 OR PD<19980403 OR AD
L25           848 L9 (L) PREP+NT/RL
L26           641 L25 AND (PY<=1998 OR AY<=1998 OR PRY<=1998 OR PD<19980403 OR AD
L27           124 L26 AND P/DT AND US/PC
L28            60 L26 AND P/DT AND US/PC.B

=> b hcap
FILE 'HCAPLUS' ENTERED AT 14:40:22 ON 22 SEP 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)


Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.
The CA Lexicon is the copyrighted intellectual property of the
the American Chemical Society and is provided to assist you in searching
databases on STN.  Any dissemination, distribution, copying, or storing
of this information, without the prior written consent of CAS, is
strictly prohibited.

FILE COVERS 1907 - 22 Sep 2004  VOL 141 ISS 13
FILE LAST UPDATED: 21 Sep 2004  (20040921/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


=> d all fhitstr l20 tot

L20  ANSWER 1 OF 2  HCAPLUS  COPYRIGHT 2004 ACS on STN
AN   2003:368618  HCAPLUS
DN   138:368624
ED   Entered STN:  14 May 2003
TI   Convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic
     acids and isoxazoles.
IN   Zhou, Jiacheng; Oh, Lynette May; Ma, Philip
PA   Bristol-Myers Squibb Pharma Company, USA
SO   U.S., 20 pp.
     CODEN: USXXAM
```

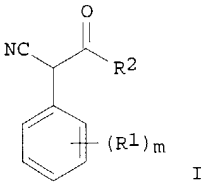
DT Patent
LA English
IC ICM C07D295-033
ICS C07D241-04; C07D211-60; C07D207-06; C07C253-12
NCL 544059000; 558355000; 558309000; 544159000; 544163000; 544399000; 546230000; 548579000
CC 25-20 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6562965	B1	20030513	US 2000-610819	20000706
	US 2003208068	A1	20031106	US 2003-387759	20030313
	US 6727360	B2	20040427		
	US 2004171829	A1	20040902	US 2004-786992	20040225
PRAI	US 1998-80680P	P	19980403		
	US 1999-282508	A3	19990331		
	US 2000-610819	A3	20000706		
	US 2003-387759	A3	20030313		

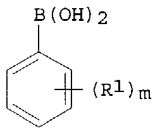
CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 6562965	ICM	C07D295-033
	ICS	C07D241-04; C07D211-60; C07D207-06; C07C253-12
	NCL	544059000; 558355000; 558309000; 544159000; 544163000; 544399000; 546230000; 548579000
US 6562965	ECLA	C07C255/41
US 2003208068	ECLA	C07C253/00; C07C255/41; C07D201/08; C07D261/08; C07D261/10B

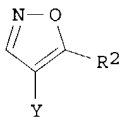
OS CASREACT 138:368624; MARPAT 138:368624
GI



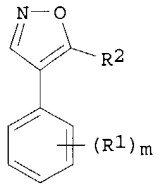
I



II



III



IV

AB .alpha.-Aryl-.beta.-ketonitriles [I; m = 0-4; R1 = H, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, amino, OH, SH, etc.; R2 = H, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, hydroxyalkyl, haloalkyl, (substituted) alkyl], which serve as synthetic intermediates in the preparation of biol. important mols. such as corticotropin releasing factor (CRF) receptor antagonists, were prepared via reaction of arylboronic acids (II; variables as above) with isoxazoles (III; Y = halo) followed by base treatment of the coupling products (IV; variables as above). Thus, 4-iodo-5-methylisoxazole (preparation given), 2,5-dimethyl-4-methoxybenzeneboronic acid (preparation given), NaHCO3, and [1,1'-bis(diphenylphosphino)ferrocene]palladium dichloride were heated in DME/H2O to give 81.1% 4-(2,5-dimethyl-4-methoxyphenyl)-5-methylisoxazole. The latter was stirred with NaOMe in MeOH to give 92% .alpha.-acetyl-.alpha.-(2,5-dimethyl-4-methoxyphenyl)acetonitrile.
ST arylketonitrile convergent synthesis; nitrile arylketo convergent synthesis
IT Nitriles, preparation
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(oxo; convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)
IT 72287-26-4, [1,1'-Bis(diphenylphosphino)ferrocene]palladium dichloride

Searched by Noble Jarrell

RL: CAT (Catalyst use); USES (Uses)
(convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)

IT **246023-57-4P 246023-58-5P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)

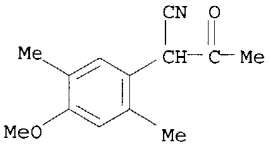
IT 1706-11-2, 2,5-Dimethylanisole 5765-44-6, 5-Methylisoxazole 27060-75-9, 4-Bromo-3-methylanisole
RL: RCT (Reactant); RACT (Reactant or reagent)
(convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)

IT 7064-37-1P, 4-Bromo-5-Methylisoxazole 7064-38-2P, 4-Iodo-5-methylisoxazole 58106-25-5P, 4-Bromo-2,5-Dimethylanisole 208399-66-0P, 4-Methoxy-2-methylbenzeneboronic acid 246023-54-1P, 2,5-Dimethyl-4-methoxybenzeneboronic acid **246023-55-2P 246023-56-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)

RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) de Munno, A; J Chem Soc, Perkin Trans 2 1977, 9, P1121 HCAPLUS
(2) Dominguez, E; J Org Chem 1966, V61, P5435
(3) Hiroyuki, Y; Chemical Abstracts 1959, V53(22)
(4) Hiroyuki, Y; Yakugaku Zasshi 1959, V79, P623
(5) Labadie, S; Synthetic Communications 1994, V24(5), P709 HCAPLUS
(6) Larock, R; Comprehensive organic transformations 1970, P57
(7) Mitchell, R; J Org Chem 1979, V44, P4733 HCAPLUS
(8) Olah, G; J Org Chem 1993, V58, P3894
(9) Olah, G; Journal of Organic Chemistry 1993, V58, P3194 HCAPLUS
(10) Rouiller, C; Heterocyclic Compounds-More than One Hetero Atom 1962, P3465
(11) Sakakibara, T; Chem Express 1989, V4, P85 HCAPLUS
(12) Sumimoto; US 4797492 A 1989 HCAPLUS
(13) Zhou; US 6107508 A 2000 HCAPLUS

IT **246023-57-4P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)

RN 246023-57-4 HCAPLUS
CN Benzeneacetonitrile, .alpha.-acetyl-4-methoxy-2,5-dimethyl- (9CI) (CA INDEX NAME)

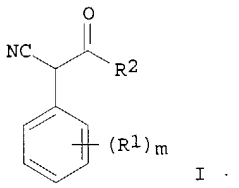


L20 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:659354 HCAPLUS
DN 131:286268
ED Entered STN: 15 Oct 1999
TI Convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles.
IN Zhou, Jicheng; **Oh, Lynette May; Ma, Philip**
PA Du Pont Pharmaceuticals Company, USA
SO PCT Int. Appl., 64 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07C253-00
CC 25-20 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
FAN.CNT 2

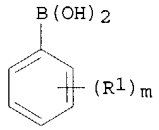
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9951568	A2	19991014	WO 1999-US6822	19990329
	WO 9951568	A3	19991118		

W: AU, BR, CA, CN, CZ, EE, HU, IL, IN, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SK, UA, VN, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

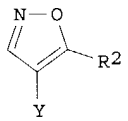
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
CA 2326846 AA 19991014 CA 1999-2326846 19990329
AU 9932135 A1 19991025 AU 1999-32135 19990329
BR 9909427 A 20001121 BR 1999-9427 19990329
EP 1066250 A2 20010110 EP 1999-914246 19990329
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO
EE 200000580 A 20020215 EE 2000-580 19990329
JP 2002510670 T2 20020409 JP 2000-542290 19990329
US 6107508 A 20000822 US 1999-282508 19990331
ZA 2000004654 A 20011011 ZA 2000-4654 20000905
NO 2000004956 A 20001101 NO 2000-4956 20001002
PRAI US 1998-80680P P 19980403
WO 1999-US6822 W 19990329
CLASS
PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES
WO 9951568 ICM C07C253-00
WO 9951568 ECLA C07C253/00; C07D201/08
OS CASREACT 131:286268; MARPAT 131:286268
GI



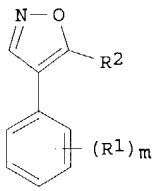
I



II



III



IV

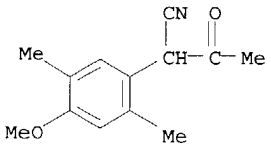
AB Title compds. [I; m = 0-4; R1 = H, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, amino, OH, SH, etc.; R2 = H, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, hydroxyalkyl, haloalkyl, (substituted) alkyl], were prepared via reaction of arylboronic acids (II; variables as above) with isoxazoles (III; Y = halo) followed by base treatment of the coupling products (IV; variables as above). Thus, 4-iodo-5-methylisoxazole (preparation given), 2,5-dimethyl-4-methoxybenzeneboronic acid (preparation given), NaHCO3, and [1,1'-bis(diphenylphosphino)ferrocene]palladium dichloride were heated in DME/H2O to give 81.1% 4-(2,5-dimethyl-4-methoxyphenyl)-5-methylisoxazole. The latter was stirred with NaOMe in MeOH to give 92% .alpha.-acetyl-.alpha.-(2,5-dimethyl-4-methoxyphenyl)acetonitrile.
ST arylketonitrile convergent synthesis; nitrile arylketo convergent synthesis
IT Nitriles, preparation
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(oxo; convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)
IT 72287-26-4, [1,1'-Bis(diphenylphosphino)ferrocene]palladium dichloride
RL: CAT (Catalyst use); USES (Uses)
(convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)
IT **246023-57-4P 246023-58-5P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)
IT 1706-11-2, 2,5-Dimethylanisole 5765-44-6, 5-Methylisoxazole 7064-37-1,

4-Bromo-5-Methylisoxazole 7064-38-2, 4-Iodo-5-methylisoxazole 27060-75-9, 4-Bromo-3-methylanisole
RL: RCT (Reactant); RACT (Reactant or reagent)
(convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)

IT 58106-25-5P, 4-Bromo-2,5-Dimethylanisole 208399-66-0P, 4-Methoxy-2-methylbenzeneboronic acid 246023-54-1P, 2,5-Dimethyl-4-methoxybenzeneboronic acid **246023-55-2P 246023-56-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)

IT **246023-57-4P**
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)

RN 246023-57-4 HCAPLUS
CN Benzeneacetonitrile, .alpha.-acetyl-4-methoxy-2,5-dimethyl- (9CI) (CA INDEX NAME)



=> d all fhitstr l22 tot

L22 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:813420 HCAPLUS
DN 135:344507
ED Entered STN: 08 Nov 2001
TI Preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists
IN He, Liqi; Gilligan, Paul; Chorvat, Robert; Arvanitis, Argyrios Georgios
PA **Dupont** Pharmaceuticals Company, USA
SO U.S., 57 pp., Cont.-in-part of U.S. Ser. No. 899,242.
CODEN: USXXAM
DT Patent
LA English
IC A61K031-535; C07D487-04
NCL 514246000
CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 2, 63
FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6313124	B1	20011106	US 1998-14734	19980128
	US 6124289	A	20000926	US 1997-899242	19970723
	ZA 9706603	A	19990125	ZA 1997-6603	19970724
	US 6136809	A	20001024	US 1998-14999	19980128
	LT 4680	B	20000725	LT 1999-8	19990125
	CA 2314613	AA	19990805	CA 1999-2314613	19990128
	WO 9938868	A1	19990805	WO 1999-US1824	19990128
	W: AU, BR, CA, CN, CZ, EE, HU, IL, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	AU 9924787	A1	19990816	AU 1999-24787	19990128
	AU 748818	B2	20020613		
	EP 1049699	A1	20001108	EP 1999-904382	19990128
	EP 1049699	B1	20040421		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
	BR 9908206	A	20001205	BR 1999-8206	19990128
	JP 2002501922	T2	20020122	JP 2000-529335	19990128
	NZ 505079	A	20030829	NZ 1999-505079	19990128
	EP 1344779	A1	20030917	EP 2003-75887	19990128
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				

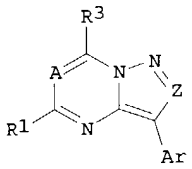
	AT 264860	E	20040515	AT 1999-904382	19990128
	TW 520372	B	20030211	TW 1999-88102636	19990223
	US 2003008885	A1	20030109	US 2001-930782	20010816
PRAI	US 1996-23290P	P	19960724		
	US 1997-899242	A2	19970723		
	US 1998-14734	A	19980128		
	US 1998-15001	A	19980128		
	US 1998-15002	A	19980128		
	EP 1999-904382	A3	19990128		
	WO 1999-US1824	W	19990128		

CLASS

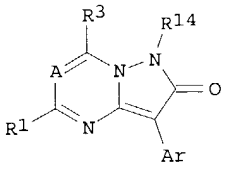
PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 6313124	IC	A61K031-535IC C07D487-04
	NCL	514246000
EP 1344779	ECLA	C07D487/04; C07D487/04
US 2003008885	ECLA	C07D487/04; C07D487/04; C07D487/04

OS MARPAT 135:344507

GI



I



II

AB The title compds. [I or II; A = N, CR; Z = N, CR2; Ar = (un)substituted Ph, naphthyl, pyridyl, etc.; R = H, alkyl, alkenyl, etc.; R1 = H, alkyl, alkenyl, etc.; R2 = H, alkyl, alkenyl, etc.; R3 = H, SH, OH, etc.; R14 = C1-10 alkyl, C3-10 alkenyl, C3-10 alkynyl, etc.], corticotropin releasing factor (CRF) antagonists (no data) which are useful in treating anxiety, depression, and other psychiatric, neurol. disorders as well as in treatment of immunol., cardiovascular or heart-related diseases and colonic hypersensitivity associated with psychopathol. disturbance and stress, were prepared and formulated. Thus, treatment of 2,7-dimethyl-8-(2,4-dimethylphenyl)[1,5-a]pyrazolo-1,3,5-triazin-4-one with POCl3 and N,N-dimethylaniline, followed by reaction of the resulting 4-chloro-2,7-dimethyl-8-(2,4-dichlorophenyl)[1,5-a]pyrazolo-1,3,5-triazine with 1,3-dimethoxy-2-aminopropane in EtOH afforded I [A = N; Z = C(Me); R1 = Me; R3 = NHCH(CH2OMe)2; Ar = 2,4-Cl2C6H3].

ST CRF antagonist azolotriazine azolopyrimidine prepn formulation; corticotropin releasing factor antagonist azolotriazine azolopyrimidine prepn

IT Corticotropin releasing factor receptors
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)
(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

IT 202578-49-2P 202579-55-3P 202579-56-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

IT

202578-50-5P	202578-51-6P	202578-52-7P	202578-53-8P	202578-54-9P
202578-55-0P	202578-57-2P	202578-58-3P	202578-59-4P	202578-60-7P
202578-61-8P	202578-62-9P	202578-63-0P	202578-64-1P	202578-65-2P
202578-66-3P	202578-67-4P	202578-68-5P	202578-69-6P	202578-70-9P
202578-71-0P	202578-72-1P	202578-73-2P	202578-74-3P	202578-75-4P
202578-76-5P	202578-77-6P	202578-78-7P	202578-79-8P	202578-80-1P
202578-81-2P	202578-82-3P	202578-83-4P	202578-84-5P	202578-85-6P
202578-86-7P	202578-88-9P	202578-90-3P	202578-92-5P	202578-93-6P
202578-94-7P	202578-95-8P	202578-96-9P	202578-97-0P	202578-98-1P
202578-99-2P	202579-00-8P	202579-01-9P	202579-02-0P	202579-03-1P
202579-04-2P	202579-05-3P	202579-06-4P	202579-08-6P	202579-10-0P
202579-12-2P	202579-14-4P	202579-16-6P	202579-18-8P	202579-20-2P
202579-22-4P	202579-23-5P	202579-25-7P	202579-27-9P	202579-29-1P
202579-30-4P	202579-32-6P	202579-34-8P	202579-36-0P	202579-38-2P
202579-39-3P	202579-41-7P	202579-43-9P	202579-45-1P	202579-46-2P
202579-47-3P	202579-48-4P	202579-49-5P	202579-50-8P	202579-51-9P

202579-52-0P 202579-53-1P 202579-54-2P 202579-57-5P 202579-58-6P
202579-59-7P 202579-60-0P 202579-61-1P 202579-62-2P 202579-63-3P
202579-64-4P 202579-65-5P 202579-66-6P 202579-68-8P 202579-69-9P
202579-70-2P 202579-71-3P 202579-72-4P 202579-73-5P 202579-74-6P
202579-75-7P 202579-76-8P 202579-77-9P 202579-78-0P 202579-79-1P
202579-80-4P 202579-81-5P 202579-82-6P 202579-83-7P 202579-84-8P
202579-85-9P 202579-86-0P 202579-87-1P 202579-88-2P 202579-89-3P
202579-90-6P 202579-91-7P 202579-92-8P 202579-93-9P 202579-94-0P
202579-95-1P 202579-96-2P 202579-97-3P 202579-98-4P 202579-99-5P
202580-00-5P 202580-01-6P 202580-02-7P 202580-03-8P 202580-04-9P
202580-05-0P 202580-06-1P 202580-07-2P 202580-08-3P 202580-09-4P
202580-10-7P 202580-11-8P 202580-12-9P 202580-13-0P 202580-14-1P
202580-15-2P 202580-16-3P 202580-17-4P 202580-18-5P 202580-19-6P
202580-20-9P 202580-21-0P 202580-22-1P 202580-23-2P 202580-24-3P
202580-25-4P 202580-26-5P 202580-27-6P 202580-28-7P 202580-29-8P
261966-75-0P 262297-98-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

IT 105-53-3, Diethyl malonate 141-97-9, Ethyl acetoacetate 616-24-0, 3-Pentylamine 622-79-7, Benzyl azide 1000-84-6 1445-45-0, Trimethyl orthoacetate 34688-71-6, 2,4,6-Trimethylbenzyl cyanide 68429-53-8, 2,4-Dimethylphenylacetonitrile 78531-29-0 202580-72-1 202580-73-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

IT **202580-61-8P**, 1-Cyano-1-(2,4-dimethylphenyl)propan-2-one
202580-62-9P, 5-Amino-4-(2,4-dimethylphenyl)-3-methylpyrazole
202580-64-1P 202580-66-3P 202580-68-5P 202580-70-9P 234778-65-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

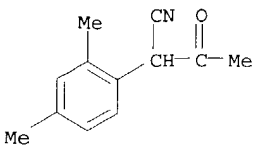
RE.CNT 103 THERE ARE 103 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Anon; 1967 HCAPLUS
(2) Anon; JP 4211753 1967
(3) Anon; 1968 HCAPLUS
(4) Anon; 1971 HCAPLUS
(5) Anon; 1971 HCAPLUS
(6) Anon; JP 6157587 1986
(7) Anon; EP 0269859 1988 HCAPLUS
(8) Anon; EP 0300688 1989 HCAPLUS
(9) Anon; EP 0373891 1989 HCAPLUS
(10) Anon; EP 0374448 1990 HCAPLUS
(11) Anon; EP 0395144 1990 HCAPLUS
(12) Anon; EP 0455545 1991 HCAPLUS
(13) Anon; EP 0503099 1992 HCAPLUS
(14) Anon; DE 4243279 1992 HCAPLUS
(15) Anon; WO 9210098 1992 HCAPLUS
(16) Anon; WO 9220642 1992 HCAPLUS
(17) Anon; EP 0521622 1993 HCAPLUS
(18) Anon; EP 0531901 1993 HCAPLUS
(19) Anon; EP 0576350 1993 HCAPLUS
(20) Anon; EP 0591528 1994 HCAPLUS
(21) Anon; EP 0594149 1994 HCAPLUS
(22) Anon; WO 9409017 1994 HCAPLUS
(23) Anon; WO 9413643 1994 HCAPLUS
(24) Anon; WO 9413644 1994 HCAPLUS
(25) Anon; WO 9413661 1994 HCAPLUS
(26) Anon; WO 9413676 1994 HCAPLUS
(27) Anon; WO 9413677 1994 HCAPLUS
(28) Anon; EP 0662477 1995 HCAPLUS
(29) Anon; EP 0714898 1995 HCAPLUS
(30) Anon; WO 9500507 1995 HCAPLUS
(31) Anon; WO 9511880 1995 HCAPLUS
(32) Anon; WO 9532710 1995 HCAPLUS
(33) Anon; WO 9533727 1995 HCAPLUS
(34) Anon; WO 9533750 1995 HCAPLUS
(35) Anon; WO 9534563 1995 HCAPLUS
(36) Anon; EP 0729758 1996 HCAPLUS
(37) Anon; WO 9535298 1996 HCAPLUS
(38) Anon; WO 9619452 1996 HCAPLUS
(39) Anon; WO 9623783 1996 HCAPLUS

(40) Anon; WO 9635689 1996 HCAPLUS
(41) Anon; WO 9639388 1996 HCAPLUS
(42) Anon; WO 9639400 1996 HCAPLUS
(43) Anon; EP 0773023 1997 HCAPLUS
(44) Anon; EP 0778277 1997 HCAPLUS
(45) Anon; EP 0812831 1997 HCAPLUS
(46) Anon; WO 9700868 1997 HCAPLUS
(47) Anon; WO 9714684 1997 HCAPLUS
(48) Anon; WO 9729109 1997 HCAPLUS
(49) Anon; WO 9729110 1997 HCAPLUS
(50) Anon; WO 9808821 1998 HCAPLUS
(51) Anon; WO 9808846 1998 HCAPLUS
(52) Anon; WO 9808847 1998 HCAPLUS
(53) Anon; Arch Pharm (Weinheim) 1987, V320, P487
(54) Arato; Biol Psychiatry 1989, V25, P355 MEDLINE
(55) Banki; Am J Psychiatry 1987, V144, P873 MEDLINE
(56) Bantick; US 5428044 1995 HCAPLUS
(57) Barker; US 5089499 1992 HCAPLUS
(58) Battaglia; Synapse 1987, V1, P572 HCAPLUS
(59) Berridge; Hormones and Behavior 1987, V21, P393 HCAPLUS
(60) Berridge; Regulatory Peptides 1986, V16, P83 HCAPLUS
(61) Blalock; Physiological Reviews 1989, V69(1), P1 HCAPLUS
(62) Britton; Life Sciences 1982, V31, P363 HCAPLUS
(63) Britton; Psychopharmacology 1985, V86, P170 HCAPLUS
(64) Britton; Psychopharmacology 1988, V94, P306 HCAPLUS
(65) Bussler; US 5484760 1996 HCAPLUS
(66) Courtemanche; US 5464847 1995 HCAPLUS
(67) de Souza; Corticotropin-Releasing Factor:Basic and Clinical Studies of a Neuropeptide P221
(68) de Souza; Hospital Practice 1988, P59 MEDLINE
(69) de Souza; Journal of Neuroscience 1985, V5(12), P3189 HCAPLUS
(70) Dunn; Brain Research Reviews 1990, V15, P71 HCAPLUS
(71) Eicken; US 4567263 1986 HCAPLUS
(72) France; Biol Psychiatry 1988, V23, P86 MEDLINE
(73) Gennaro; Remington's Pharmaceutical Sciences, 17th ed P1418
(74) Gold; New Eng J Med 1986, V314(21), P1329 MEDLINE
(75) Grigoriadis; Neuropsychopharmacology 1989, V2(1), P53 HCAPLUS
(76) Hashimoto; US 5137887 1992 HCAPLUS
(77) Himmelsbach; US 5463071 1995 HCAPLUS
(78) Himmler; US 4990647 1991 HCAPLUS
(79) Koob; Perspectives on Behavioral Medicine 1985, V2, P39
(80) Kruger; US 4892576 1990 HCAPLUS
(81) Maquestiau; Bull Soc Chim Belg 1992, V101(2) HCAPLUS
(82) Morley; Life Sciences 1987, V41, P527 HCAPLUS
(83) Nemeroff; Arch Gen Psychiatry 1988, V45, P577 MEDLINE
(84) Nemeroff; Science 1984, V226, P1342 MEDLINE
(85) Nugent; US 5397774 1995 HCAPLUS
(86) O'Brien; US 3910907 1975 HCAPLUS
(87) O'Brien; 1976 HCAPLUS
(88) Rivier; Proc Natl Acad Sci 1983, V80, P4851 HCAPLUS
(89) Rooney; US 3995039 1976 HCAPLUS
(90) Sapolsky; Arch Gen Psychiatry 1989, V46, P1047 MEDLINE
(91) Schonafinger; US 5486531 1996 HCAPLUS
(92) Senga; 1982 HCAPLUS
(93) Senga; J Med Chem 1982, V25, P243 HCAPLUS
(94) Senga; J Med Chem 1982, V25, P243 HCAPLUS
(95) Springer; US 3920652 1975 HCAPLUS
(96) Springer; US 4021556 1977 HCAPLUS
(97) Swerdlow; Psychopharmacology 1986, V88, P147 HCAPLUS
(98) Trost; Comprehensive Organic Synthesis V3, P481
(99) Trost; Comprehensive Organic Synthesis V7, P762
(100) Vale; Recent Progress in Hormone Research 1983, V39, P245 HCAPLUS
(101) Vale; Science 1981, V213, P1394 HCAPLUS
(102) Vinogradoff; US 4997940 1991 HCAPLUS
(103) Yuan; US 5723608 1998 HCAPLUS

IT **202580-61-8P**, 1-Cyano-1-(2,4-dimethylphenyl)propan-2-one
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

RN 202580-61-8 HCAPLUS

CN Benzeneacetonitrile, .alpha.-acetyl-2,4-dimethyl- (9CI) (CA INDEX NAME)



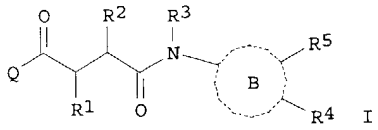
L22 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:618005 HCAPLUS
DN 135:195579
ED Entered STN: 24 Aug 2001
TI Preparation and activity of succinoylamino carbocycles and heterocycles as inhibitors of a.beta. protein production
IN Olson, Richard E.; Maduskuie, Thomas P.; Thompson, Lorin Andrew; Tebben, Andrew J.; Wang, Nenghui; Deng, Wei; Liu, Hong
PA **Dupont** Pharmaceuticals Company, USA
SO PCT Int. Appl., 236 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D487-04
ICS C07D471-04; C07D471-08; C07D243-24; A61K031-55; A61K031-551; A61K031-5513; A61K031-5517; A61P025-28; C07D487-04; C07D223-00; C07D209-00; C07D471-04; C07D223-00; C07D221-00; C07D471-08; C07D223-00; C07D221-00; C07D487-04; C07D223-00
CC 28-21 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001060826	A2	20010823	WO 2001-US5236	20010216
	WO 2001060826	A3	20020117		
	W: AU, BR, CA, CN, CZ, EE, HU, IL, IN, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, VN, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
	US 2002055501	A1	20020509	US 2001-788227	20010216
	US 6525044	B2	20030225		
	EP 1261610	A2	20021204	EP 2001-914400	20010216
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR				
	JP 2003523345	T2	20030805	JP 2001-560210	20010216
PRAI	US 2000-183186P	P	20000217		
	WO 2001-US5236	W	20010216		

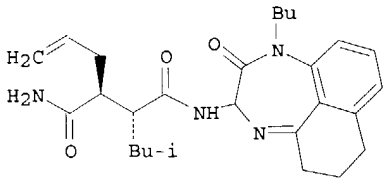
CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2001060826	ICM	C07D487-04
	ICS	C07D471-04; C07D471-08; C07D243-24; A61K031-55; A61K031-551; A61K031-5513; A61K031-5517; A61P025-28; C07D487-04; C07D223-00; C07D209-00; C07D471-04; C07D223-00; C07D221-00; C07D471-08; C07D223-00; C07D221-00; C07D487-04; C07D223-00
US 2002055501	ECLA	C07D243/24; C07D401/06; C07D471/04; C07D471/04; C07D471/06; C07D471/08; C07D487/04; C07D487/04; C07D487/06; C07D087/06

OS MARPAT 135:195579
GI



I



II

AB Synthesis of succinoylamino carbocycles and heterocycles (I) [Q = (un)substituted OH, NH2; R1 = (un)substituted alkyl, alkenyl; R2 = (un)substituted alkyl; R3 = H, alkyl; R4 = (un)substituted aryl; R5 = (un)substituted OH, (un)substituted CONH2, (un)substituted alkyl; B = nitrogen heterocycle fused by one or more (un)substituted (un)saturated carbocyclic or heterocyclic rings] having drug and bio-affecting properties, their pharmaceutical compns. and methods of use is disclosed. Thus, (II) was prepared by amidation of 2-amino-3-oxo-2,3,4,8,9,10-hexahydronaphtho[1,8-ef]diazepine with tert-Bu (2R,3S)-3-allyl-2-isobutylsuccinic acid followed by aminolysis and butylation. II inhibits production of .beta.-amyloid protein with an IC50 < 100.upsilon.M in an immunopptn. assay using N9 cells characterized for expression of exogenous amyloid precursor protein. These novel compds. inhibit the processing of amyloid precursor protein and, more specifically, inhibit the production of A.beta.-peptide, thereby acting to prevent the formation of neurol. deposits of amyloid protein. More particularly, the present invention relates to the treatment of neurol. disorders related to .beta.-amyloid production such as Alzheimer's disease and Down's Syndrome.

ST amyloid protein inhibitor succinoylamino carbocycle heterocycle

IT Anti-Alzheimer's agents
(preparation and activity of succinoylamino carbocycles and heterocycles as inhibitors of a.beta. protein production)

IT Amyloid
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(preparation and activity of succinoylamino carbocycles and heterocycles as inhibitors of a.beta. protein production)

IT Down's syndrome
(treatment of; preparation and activity of succinoylamino carbocycles and heterocycles as inhibitors of a.beta. protein production)

IT 158736-49-3, .beta. Secretase 338454-52-7, .gamma. Secretase
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(method for inhibition of; preparation and activity of succinoylamino carbocycles and heterocycles as inhibitors of a.beta. protein production)

IT 356040-26-1P 356040-27-2P 356040-34-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation and activity of succinoylamino carbocycles and heterocycles as inhibitors of a.beta. protein production)

IT 356040-12-5P 356040-13-6P 356040-14-7P 356040-15-8P 356040-16-9P
356040-17-0P 356040-18-1P 356040-19-2P 356040-20-5P 356040-21-6P
356040-22-7P 356040-23-8P 356040-24-9P 356040-25-0P 356040-28-3P
356040-29-4P 356040-30-7P 356040-31-8P 356040-32-9P
356040-33-0P 356040-35-2P 356040-36-3P 356040-78-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and activity of succinoylamino carbocycles and heterocycles as inhibitors of a.beta. protein production)

IT 356040-61-4P
RL: BYP (Byproduct); SPN (Synthetic preparation); PREP (Preparation)
(preparation and activity of succinoylamino carbocycles and heterocycles as inhibitors of a.beta. protein production)

IT 356040-76-1P 356040-77-2P
RL: PEP (Physical, engineering or chemical process); PUR (Purification or recovery); PREP (Preparation); PROC (Process)
(preparation and activity of succinoylamino carbocycles and heterocycles as inhibitors of a.beta. protein production)

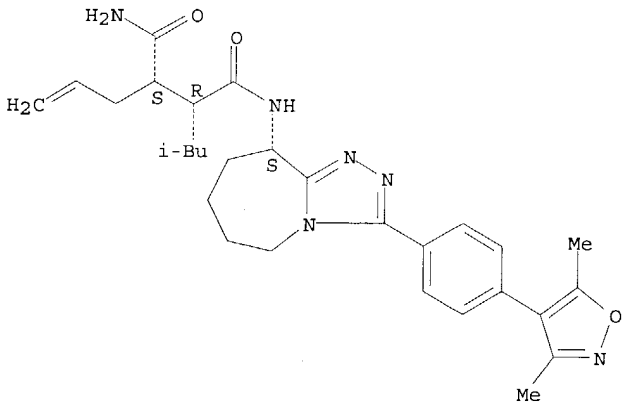
IT 62-53-3, Aniline, reactions 74-88-4, Iodomethane, reactions 75-31-0, Isopropylamine, reactions 98-80-6, Phenylboronic acid 100-46-9, Benzylamine, reactions 542-69-8, Butyl iodide 1210-35-1, Dibenzosuberone 1679-18-1, 4-Chlorophenylboronic acid 2217-41-6, 5,6,7,8-Tetrahydro-1-naphthylamine 2393-23-9, 4-Methoxybenzylamine 3218-02-8, Cyclohexanemethanamine 5071-96-5, 3-Methoxybenzylamine 5392-81-4 5933-32-4 16114-47-9 16947-84-5 33244-57-4 54631-81-1 55401-97-3, 2-(Bromomethyl)pyridine 65365-28-8, D-Proline methyl ester hydrochloride 76944-95-1 90600-20-7 98437-24-2 114715-38-7, (S)-3-Amino-1-benzylpyrrolidine 114715-39-8, (R)-3-Amino-1-benzylpyrrolidine 124676-19-3 126544-38-5 148415-75-2 204326-24-9 219615-42-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and activity of succinoylamino carbocycles and heterocycles as inhibitors of a.beta. protein production)

IT 1785-74-6P 6272-18-0P 7005-53-0P 39115-96-3P 109953-95-9P 110139-15-6P 126149-54-0P 136024-61-8P 210346-49-9P 356040-37-4P 356040-38-5P 356040-39-6P 356040-40-9P 356040-41-0P 356040-42-1P 356040-43-2P 356040-44-3P 356040-45-4DP, resin bound 356040-46-5DP, resin bound 356040-47-6P 356040-48-7P 356040-49-8P 356040-50-1P 356040-51-2P 356040-52-3P 356040-53-4P 356040-54-5P 356040-55-6P 356040-56-7P 356040-57-8P 356040-58-9P 356040-59-0P 356040-60-3P 356040-62-5P 356040-63-6P 356040-64-7P 356040-65-8P 356040-66-9P 356040-67-0P 356040-68-1P 356040-69-2P 356040-70-5P 356040-71-6P **356040-72-7P** 356040-73-8P 356040-74-9P 356040-75-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and activity of succinoylamino carbocycles and heterocycles as inhibitors of a.beta. protein production)

IT **356040-33-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and activity of succinoylamino carbocycles and heterocycles as inhibitors of a.beta. protein production)

RN 356040-33-0 HCAPLUS
CN Butanediamide, N1-[(9S)-3-[4-(3,5-dimethyl-4-isoxazolyl)phenyl]-6,7,8,9-tetrahydro-5H-1,2,4-triazolo[4,3-a]azepin-9-yl]-2-(2-methylpropyl)-3-(2-propenyl)-, (2R,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L22 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:131201 HCAPLUS
DN 134:178572
ED Entered STN: 22 Feb 2001
TI Preparation of azolo triazines and pyrimidines as corticotropin releasing factor (CRF) antagonists
IN He, Liqi; Gilligan, Paul; Chorvat, Robert; Arvanitis, Argyrios Georgios
PA **Dupont** Pharmaceuticals Co., USA

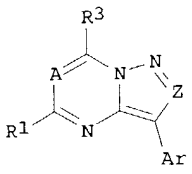
SO U.S., 90 pp., Cont.-in-part of U. S. Ser. No. 899,242.
CODEN: USXXAM
DT Patent
LA English
IC ICM C07D487-04
ICS C07D251-72; A61K031-53
NCL 514246000
CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 2, 63
FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6191131	B1	20010220	US 1998-15002	19980128
	US 6124289	A	20000926	US 1997-899242	19970723
	ZA 9706603	A	19990125	ZA 1997-6603	19970724
	US 6136809	A	20001024	US 1998-14999	19980128
	LT 4680	B	20000725	LT 1999-8	19990125
	CA 2314613	AA	19990805	CA 1999-2314613	19990128
	WO 9938868	A1	19990805	WO 1999-US1824	19990128
	W: AU, BR, CA, CN, CZ, EE, HU, IL, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	AU 9924787	A1	19990816	AU 1999-24787	19990128
	AU 748818	B2	20020613		
	EP 1049699	A1	20001108	EP 1999-904382	19990128
	EP 1049699	B1	20040421		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
	BR 9908206	A	20001205	BR 1999-8206	19990128
	JP 2002501922	T2	20020122	JP 2000-529335	19990128
	NZ 505079	A	20030829	NZ 1999-505079	19990128
	EP 1344779	A1	20030917	EP 2003-75887	19990128
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
	AT 264860	E	20040515	AT 1999-904382	19990128
	TW 520372	B	20030211	TW 1999-88102636	19990223
	US 6358950	B1	20020319	US 2000-696759	20001026
PRAI	US 1996-23290P	P	19960724		
	US 1997-899242	A2	19970723		
	US 1998-14734	A	19980128		
	US 1998-15001	A	19980128		
	US 1998-15002	A	19980128		
	EP 1999-904382	A3	19990128		
	WO 1999-US1824	W	19990128		

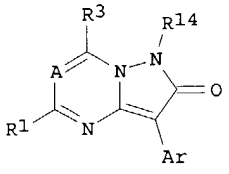
CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 6191131	ICM	C07D487-04
	ICS	C07D251-72; A61K031-53
	NCL	514246000
EP 1344779	ECLA	C07D487/04; C07D487/04

OS MARPAT 134:178572
GI



I



II

AB The title compds. [I or II; A = N, CR; Z = N, CR2; Ar = (un)substituted Ph, naphthyl, pyridyl, etc.; R = H, alk(en/yn)yl, halo, etc.; R1, R2 = H, alk(en/yn)yl, halo, etc.; R3 = H, SH, aryl, etc.; R14 = (un)substituted alk(en/yn)yl, cycloalkyl(alkyl)], useful in treating CRF-related disorders, particularly anxiety, depression, and other psychiatric, neurol. disorders as well as treatment of immunol., cardiovascular or heart-related diseases and colonic hypersensitivity associated with psychopathol. disturbance and stress, were prepared and formulated. For

instance, 5-amino-4-(2-chloro-4-methylphenyl)-3-methylpyrazole was cyclized with Et acetoacetate in AcOH to give 42% 7-hydroxy-2,5-dimethyl-3-(2-chloro-4-methylphenyl)pyrazolo[1,5-a]pyrimidine. The latter was treated with POCl3 and PhNEt2 to give the 7-chloro analog (84%), which reacted with 3-pentylamine to give 60% title compound I [A = CH; R1 = Me; R3 = NHCHEt2; Z = CMe; Ar = 2-Cl-4-MeC6H3]. The compds. I are effective at 0.002-200 mg/kg/day.

ST azolo triazine pyrimidine prepn formulation CRF antagonist; corticotropin releasing factor antagonist pyrazolopyrimidine pyrazolotriazine prepn antidepressant anxiolytic; azolotriazine prepn formulation CRF receptor antagonist; azolopyrimidine prepn formulation CRF receptor antagonist

IT Antidepressants
Anxiolytics
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT Corticotropin releasing factor receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT 202578-49-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT
202578-50-5P	202578-51-6P	202578-52-7P	202578-53-8P	202578-54-9P
202578-55-0P	202578-58-3P	202578-59-4P	202578-60-7P	202578-61-8P
202578-62-9P	202578-63-0P	202578-64-1P	202578-65-2P	202578-66-3P
202578-67-4P	202578-68-5P	202578-69-6P	202578-70-9P	202578-71-0P
202578-72-1P	202578-73-2P	202578-74-3P	202578-75-4P	202578-76-5P
202578-77-6P	202578-78-7P	202578-79-8P	202578-80-1P	202578-81-2P
202578-82-3P	202578-83-4P	202578-84-5P	202578-85-6P	202578-86-7P
202578-88-9P	202578-90-3P	202578-92-5P	202578-93-6P	202578-94-7P
202578-95-8P	202578-96-9P	202578-97-0P	202578-98-1P	202578-99-2P
202579-00-8P	202579-01-9P	202579-02-0P	202579-03-1P	202579-04-2P
202579-05-3P	202579-06-4P	202579-08-6P	202579-10-0P	202579-12-2P
202579-14-4P	202579-16-6P	202579-18-8P	202579-20-2P	202579-22-4P
202579-23-5P	202579-25-7P	202579-27-9P	202579-29-1P	202579-30-4P
202579-32-6P	202579-34-8P	202579-36-0P	202579-38-2P	202579-39-3P
202579-41-7P	202579-43-9P	202579-45-1P	202579-46-2P	202579-47-3P
202579-48-4P	202579-49-5P	202579-50-8P	202579-51-9P	202579-52-0P
202579-53-1P	202579-54-2P	202579-55-3P	202579-56-4P	202579-57-5P
202579-58-6P	202579-59-7P	202579-60-0P	202579-61-1P	202579-62-2P
202579-63-3P	202579-64-4P	202579-65-5P	202579-66-6P	202579-68-8P
202579-69-9P	202579-70-2P	202579-71-3P	202579-72-4P	202579-73-5P
202579-74-6P	202579-75-7P	202579-76-8P	202579-77-9P	202579-78-0P
202579-79-1P	202579-80-4P	202579-81-5P	202579-82-6P	202579-83-7P
202579-84-8P	202579-85-9P	202579-86-0P	202579-87-1P	202579-88-2P
202579-89-3P	202579-90-6P	202579-91-7P	202579-92-8P	202579-93-9P
202579-94-0P	202579-95-1P	202579-96-2P	202579-97-3P	202579-98-4P
202579-99-5P	202580-00-5P	202580-01-6P	202580-02-7P	202580-04-9P
202580-05-0P	202580-06-1P	202580-07-2P	202580-08-3P	202580-09-4P
202580-10-7P	202580-11-8P	202580-12-9P	202580-13-0P	202580-14-1P
202580-15-2P	202580-16-3P	202580-17-4P	202580-18-5P	202580-19-6P
202580-20-9P	202580-21-0P	202580-22-1P	202580-23-2P	202580-24-3P
202580-25-4P	202580-26-5P	202580-27-6P	202580-28-7P	202580-29-8P
202580-30-1P	202580-32-3P	202580-35-6P	202580-36-7P	202580-37-8P
202580-38-9P	202580-39-0P	202580-40-3P	202580-41-4P	234772-66-8P
234772-67-9P	234772-68-0P	234772-69-1P	234772-70-4P	234772-71-5P
234772-72-6P	234772-73-7P	234772-74-8P	234772-75-9P	234772-76-0P
234772-77-1P	234772-78-2P	234772-79-3P	234772-80-6P	234772-81-7P
234772-82-8P	234772-83-9P	234772-84-0P	234772-86-2P	234772-87-3P
234772-88-4P	234772-89-5P	234772-90-8P	234772-91-9P	234772-92-0P
234772-93-1P	234772-94-2P	234772-95-3P	234772-96-4P	234772-97-5P
234772-98-6P	234772-99-7P	234773-00-3P	234773-01-4P	234773-02-5P
234773-03-6P	234773-04-7P	234773-05-8P	234773-07-0P	234773-09-2P
234773-11-6P	234773-13-8P	234773-15-0P	234773-16-1P	234773-18-3P
234773-19-4P	234773-20-7P	234773-21-8P	234773-22-9P	234773-23-0P
234773-24-1P	234773-25-2P	234773-26-3P	234773-27-4P	234773-29-6P
234773-31-0P	234773-33-2P	234773-35-4P	234773-37-6P	234773-38-7P
234773-40-1P	234773-42-3P	234773-44-5P	234773-46-7P	234773-48-9P
234773-50-3P	234773-51-4P	234773-52-5P	234773-53-6P	

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT
234773-54-7P	234773-56-9P	234773-58-1P	234773-60-5P	234773-62-7P

234773-64-9P 234773-66-1P 234773-68-3P 234773-70-7P 234773-72-9P
234773-74-1P 234773-75-2P 234773-76-3P 234773-77-4P 234773-78-5P
234773-79-6P 234773-80-9P 234773-81-0P 234773-82-1P 234773-83-2P
234773-84-3P 234773-85-4P 234773-86-5P 234773-87-6P 234773-88-7P
234773-89-8P 234773-90-1P 234773-91-2P 234773-92-3P 234773-93-4P
234773-94-5P 234773-95-6P 234773-96-7P 234773-97-8P 234773-98-9P
234773-99-0P 234774-00-6P 234774-01-7P 234774-02-8P 234774-03-9P
234774-04-0P 234774-05-1P 234774-06-2P 234774-07-3P 234774-08-4P
234774-09-5P 234774-10-8P 234774-11-9P 234774-12-0P 234774-13-1P
234774-14-2P 234774-15-3P 234774-16-4P 234774-17-5P 234774-18-6P
234774-19-7P 234774-20-0P 234774-21-1P 234774-22-2P 234774-23-3P
234774-24-4P 234774-25-5P 234774-26-6P 234774-27-7P 234774-28-8P
234774-29-9P 234774-30-2P 234774-31-3P 234774-32-4P 234774-33-5P
234774-34-6P 234774-35-7P 234774-36-8P 234774-37-9P 234774-38-0P
234774-39-1P 234774-40-4P 234774-41-5P 234774-42-6P 234774-43-7P
234774-44-8P 234774-45-9P 234774-46-0P 234774-47-1P 234774-48-2P
234774-49-3P 234774-50-6P 234774-51-7P 234774-52-8P 234774-53-9P
234774-54-0P 234774-55-1P 234774-57-3P 234774-59-5P 234774-61-9P
234774-63-1P 234774-64-2P 234774-65-3P 234774-66-4P 234774-67-5P
234774-69-7P 234774-74-4P 234774-76-6P 234774-78-8P 234774-80-2P
234774-82-4P 234774-84-6P 234774-86-8P 234774-88-0P 234774-89-1P
234774-91-5P 234774-92-6P 234774-93-7P 234774-94-8P 234774-95-9P
234774-96-0P 234774-97-1P 234774-98-2P 234774-99-3P 234775-00-9P
234775-01-0P 234775-02-1P 234775-03-2P 234775-04-3P 234775-05-4P
234775-06-5P 234775-07-6P 234775-08-7P 234775-09-8P 234775-10-1P
234775-11-2P 234775-12-3P 234775-13-4P 234775-14-5P 234775-16-7P
234775-17-8P 234775-18-9P 234775-19-0P 234775-20-3P 234775-21-4P
234775-22-5P 234775-23-6P 234775-24-7P 234775-25-8P 234775-26-9P
234775-27-0P 234775-28-1P 234775-29-2P 234775-30-5P 234775-31-6P
234775-32-7P 234775-33-8P 234775-34-9P 234775-35-0P 234775-36-1P
234775-37-2P 234775-38-3P 234775-39-4P 234775-40-7P 234775-41-8P
234775-42-9P 234775-43-0P 234775-44-1P 234775-45-2P 234775-46-3P
234775-47-4P 234775-48-5P 234775-49-6P 234775-50-9P 234775-51-0P
234775-52-1P 234775-53-2P 234775-54-3P 234775-55-4P 234775-56-5P
234775-57-6P 234775-58-7P 234775-59-8P 234775-60-1P 234775-61-2P
234775-62-3P 234775-63-4P 234775-64-5P 234775-65-6P 234775-66-7P
234775-67-8P 234775-68-9P 234775-69-0P 234775-70-3P 234775-71-4P
234775-72-5P 234775-73-6P 234775-74-7P 234775-76-9P 234775-77-0P
234775-78-1P 234775-79-2P 234775-80-5P 234775-81-6P 234775-82-7P
234775-83-8P 234775-84-9P 234775-85-0P 234775-86-1P 234775-87-2P
234775-88-3P 234775-89-4P 234775-90-7P 234775-91-8P 234775-92-9P
234775-93-0P 234775-94-1P 234775-95-2P 234775-96-3P 234775-97-4P
234775-98-5P 234775-99-6P 234776-00-2P 234776-01-3P 234776-02-4P
234776-03-5P 234776-04-6P 234776-05-7P 234776-06-8P 234776-07-9P
234776-08-0P 234776-09-1P 234776-10-4P 234776-11-5P 234776-12-6P
234776-13-7P 234776-14-8P 234776-15-9P 234776-16-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT 234776-17-1P 234776-18-2P 234776-19-3P 234776-20-6P 234776-21-7P
234776-22-8P 234776-23-9P 234776-24-0P 234776-26-2P 234776-27-3P
234776-28-4P 234776-29-5P 234776-30-8P 234776-31-9P 234776-32-0P
234776-33-1P 234776-34-2P 234776-35-3P 234776-36-4P 234776-37-5P
234776-38-6P 234776-39-7P 234776-40-0P 234776-41-1P 234776-42-2P
234776-43-3P 234776-44-4P 234776-45-5P 234776-46-6P 234776-47-7P
234776-48-8P 234776-49-9P 234776-50-2P 234776-51-3P 234776-52-4P
234776-53-5P 234776-54-6P 234776-55-7P 234776-56-8P 234776-57-9P
234776-58-0P 234776-59-1P 234776-60-4P 234776-61-5P 234776-62-6P
234776-63-7P 234776-64-8P 234776-65-9P 234776-66-0P 234776-67-1P
234776-68-2P 234776-69-3P 234778-55-3P 234778-56-4P 234778-57-5P
234778-58-6P 234778-59-7P 234778-60-0P 234778-61-1P 261966-75-0P
326821-49-2P 326821-82-3P 326821-83-4P 326821-84-5P 326821-85-6P
326821-86-7P 326821-87-8P 326821-88-9P 326821-89-0P 326821-90-3P
326821-91-4P 326821-93-6P 326821-94-7P 326821-95-8P 326821-96-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT 105-53-3, Diethyl malonate 105-58-8, Diethyl carbonate 141-97-9, Ethyl acetoacetate 616-24-0, 3-Pentylamine 622-79-7, Benzyl azide
1445-45-0, Trimethyl orthoacetate 2208-07-3 34688-71-6, 2,4,6-Trimethylbenzyl cyanide 68429-53-8, 2,4-Dimethylphenylacetonitrile
78531-29-0 202580-72-1 202580-73-2 326821-97-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT 1000-84-6P **202580-61-8P** 202580-62-9P 202580-64-1P
202580-66-3P 202580-68-5P 202580-70-9P 234778-65-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

RE.CNT 93 THERE ARE 93 CITED REFERENCES AVAILABLE FOR THIS RECORD

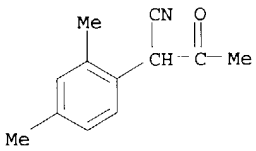
RE

(1) Anon; 1967, 28, HCAPLUS
(2) Anon; JP 4211753 1967
(3) Anon; 1968, 28, HCAPLUS
(4) Anon; 1971, 28, HCAPLUS
(5) Anon; 1971, 28, HCAPLUS
(6) Anon; JP 6157587 1986
(7) Anon; EP 0269859 1988 HCAPLUS
(8) Anon; EP 0300688 1989 HCAPLUS
(9) Anon; EP 0373891 1989 HCAPLUS
(10) Anon; EP 0374448 1990 HCAPLUS
(11) Anon; EP 0395144 1990 HCAPLUS
(12) Anon; EP 0455545 1991 HCAPLUS
(13) Anon; EP 0503099 1992 HCAPLUS
(14) Anon; WO 9220642 1992 HCAPLUS
(15) Anon; EP 0521622 1993 HCAPLUS
(16) Anon; EP 0531901 1993 HCAPLUS
(17) Anon; EP 0576350 1993 HCAPLUS
(18) Anon; EP 0591528 1994 HCAPLUS
(19) Anon; EP 0594149 1994 HCAPLUS
(20) Anon; WO 9409017 1994 HCAPLUS
(21) Anon; WO 9413643 1994 HCAPLUS
(22) Anon; WO 9413644 1994 HCAPLUS
(23) Anon; WO 9413661 1994 HCAPLUS
(24) Anon; WO 9413676 1994 HCAPLUS
(25) Anon; WO 9413677 1994 HCAPLUS
(26) Anon; EP 0662477 1995 HCAPLUS
(27) Anon; EP 0714898 1995 HCAPLUS
(28) Anon; WO 9500507 1995 HCAPLUS
(29) Anon; WO 9511880 1995 HCAPLUS
(30) Anon; WO 9533727 1995 HCAPLUS
(31) Anon; WO 9533750 1995 HCAPLUS
(32) Anon; WO 9534563 1995 HCAPLUS
(33) Anon; EP 0729758 1996 HCAPLUS
(34) Anon; WO 9535298 1996 HCAPLUS
(35) Anon; WO 9619452 1996 HCAPLUS
(36) Anon; WO 9623783 1996 HCAPLUS
(37) Anon; WO 9635689 1996 HCAPLUS
(38) Anon; WO 9639388 1996 HCAPLUS
(39) Anon; WO 9639400 1996 HCAPLUS
(40) Anon; EP 0773023 1997 HCAPLUS
(41) Anon; EP 0778277 1997 HCAPLUS
(42) Anon; EP 0812831 1997 HCAPLUS
(43) Anon; Remington's Pharmaceutical Sciences 17th P1418
(44) Arato; Biol Psychiatry 1989, V25, P355 MEDLINE
(45) Baker; US 5089499 1992 HCAPLUS
(46) Banki; Am J Psychiatry 1987, V144, P873 MEDLINE
(47) Bantick; US 5428044 1995 HCAPLUS
(48) Battaglia; Synapse 1987, V1, P572 HCAPLUS
(49) Berridge; Hormones and Behavior 1987, V21, P393 HCAPLUS
(50) Berridge; Regulatory Peptides 1986, V16, P83 HCAPLUS
(51) Blalock; Physiological Reviews 1989, V69(1), P1 HCAPLUS
(52) Britton; Life Sciences 1982, V31, P363 HCAPLUS
(53) Britton; Psychopharmacology 1985, V86, P170 HCAPLUS
(54) Britton; Psychopharmacology 1988, V94, P306 HCAPLUS
(55) Bussler; US 5484760 1996 HCAPLUS
(56) De Souza; Corticotropin Releasing Factor: Basic and Clinical Studies of a Neuropeptide 1990, P221
(57) De Souza; Hospital Practice 1988, P59 MEDLINE
(58) De Souza; Journal of Neuroscience 1985, V5(12), P3189 HCAPLUS
(59) Dunn; Brain Research Reviews 1990, V15, P71 HCAPLUS
(60) Eicken; US 4567263 1986 HCAPLUS
(61) France; Biol Psychiatry 1988, V23, P86 MEDLINE
(62) Gold; New Eng J Med 1986, V314(21), P1329 MEDLINE
(63) Grigoriadis; Neuropsychopharmacology 1989, V2(1), P53 HCAPLUS
(64) Hashimoto; US 5137887 1992 HCAPLUS
(65) Himmelsbach; US 5463071 1995 HCAPLUS
(66) Himmler; US 4990647 1991 HCAPLUS
(67) Joshi; Journal f prakt Chemie 1979, P341 HCAPLUS
(68) Koob; Perspectives on Behavioral Medicine 1985, V2, P39

(69) Kruger; US 4892576 1990 HCAPLUS
(70) Maquestiau; Bull Soc Chim Belg 1992, V101(2) HCAPLUS
(71) Morley; Life Sciences 1987, V41, P527 HCAPLUS
(72) Nemeroff; Arch Gen Psychiatry 1988, V45, P577 MEDLINE
(73) Nemeroff; Science 1984, V226, P1342 MEDLINE
(74) Nugent; US 5397774 1995 HCAPLUS
(75) O'Brien; US 3910907 1975 HCAPLUS
(76) O'Brien; J Heterocyclic Chem 1985, V22, P601
(77) Rivier; Proc Natl Acad Sci 1983, V80, P4851 HCAPLUS
(78) Rooney; US 3995039 1976 HCAPLUS
(79) Sapolsky; Arch Gen Psychiatry 1989, V46, P1047 MEDLINE
(80) Schonafinger; US 5486531 1996 HCAPLUS
(81) Senga; J Med Chem 1981, V24, P610 HCAPLUS
(82) Senga; J Med Chem 1982, V25, P243 HCAPLUS
(83) Springer; US 3920652 1975 HCAPLUS
(84) Springer; US 4021556 1977 HCAPLUS
(85) Springer; Journal of Medicinal Chemistry 1976, V19(2), P291 HCAPLUS
(86) Swerdlow; Psychopharmacology 1986, V88, P147 HCAPLUS
(87) Trost; Comprehensive Organic Synthesis 1991, V3, P481
(88) Trost; Comprehensive Organic Synthesis 1991, V7, P762
(89) Vale; Recent Progress in Hormone Research 1983, V39, P245 HCAPLUS
(90) Vale; Science 1981, P213
(91) Vinogradoff; US 4997940 1991 HCAPLUS
(92) Weinheim; Arch Pharm 1987, V320, P487
(93) Yuan; US 5723608 1998 HCAPLUS

IT **202580-61-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

RN 202580-61-8 HCAPLUS
CN Benzeneacetonitrile, .alpha.-acetyl-2,4-dimethyl- (9CI) (CA INDEX NAME)



L22 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:307132 HCAPLUS
DN 132:321873
ED Entered STN: 12 May 2000
TI Azolo triazines and pyrimidines useful as corticotropin releasing factor (CRF) antagonists
IN Gilligan, Paul; Chorvat, Robert; Arvanitis, Argyrios Georgios
PA **DuPont** Pharmaceuticals Co., USA
SO U.S., 86 pp., Cont.-in-part of U.S. Ser. No. 899,242.
CODEN: USXXAM
DT Patent
LA English
IC ICM A61K031-505
ICS C07D487-04
NCL 514258000
CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 2

FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6060478	A	20000509	US 1998-15001	19980128
	US 6124289	A	20000926	US 1997-899242	19970723
	ZA 9706603	A	19990125	ZA 1997-6603	19970724
	US 6136809	A	20001024	US 1998-14999	19980128
	LT 4680	B	20000725	LT 1999-8	19990125
	CA 2314613	AA	19990805	CA 1999-2314613	19990128
	WO 9938868	A1	19990805	WO 1999-US1824	19990128
	W: AU, BR, CA, CN, CZ, EE, HU, IL, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	AU 9924787	A1	19990816	AU 1999-24787	19990128
	AU 748818	B2	20020613		
	EP 1049699	A1	20001108	EP 1999-904382	19990128

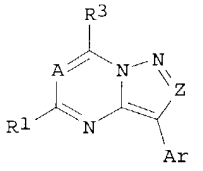
	EP 1049699	B1	20040421		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
	BR 9908206	A	20001205	BR 1999-8206	19990128
	JP 2002501922	T2	20020122	JP 2000-529335	19990128
	NZ 505079	A	20030829	NZ 1999-505079	19990128
	EP 1344779	A1	20030917	EP 2003-75887	19990128
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
	AT 264860	E	20040515	AT 1999-904382	19990128
	TW 520372	B	20030211	TW 1999-88102636	19990223
PRAI	US 1996-23290P	P	19960724		
	US 1997-899242	A2	19970723		
	US 1998-14734	A	19980128		
	US 1998-15001	A	19980128		
	US 1998-15002	A	19980128		
	EP 1999-904382	A3	19990128		
	WO 1999-US1824	W	19990128		

CLASS

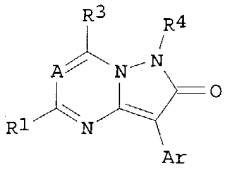
PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 6060478	ICM	A61K031-505
	ICS	C07D487-04
	NCL	514258000
US 6060478	ECLA	C07D487/04; C07D487/04; C07D487/04
EP 1344779	ECLA	C07D487/04; C07D487/04

OS MARPAT 132:321873

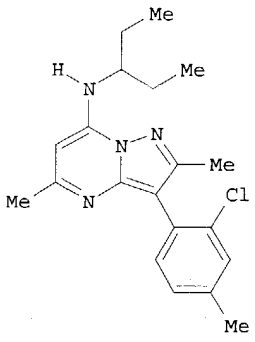
GI



I



II



III

AB Corticotropin releasing factor (CRF) antagonists (no data) of formulas I and II are disclosed [wherein A = N or CR; Z = N or CR2; Ar = (un)substituted Ph, naphthyl, pyridyl, pyrimidinyl, indanyl, tetralinyl, addnl. selected heterocycles; R = H, alk(en/yn)yl, cycloalkyl(alkyl), halo, cyano, haloalkyl; R1, R2 = H, groups listed for R, NH2 or derivs., OH or derivs., SH or derivs., addnl. substituted alkyls; R3 = H, OH or derivs., SH or derivs., acyl, CO2H or esters, NH2 or derivs., aryl, heteroaryl, alk(en/yn)yl, etc.; R4 = (un)substituted alk(en/yn)yl or cycloalkyl(alkyl)]. The compds. are of use in the treatment of CRF-related disorders, particularly anxiety and depression, as well as other psychiatric, neurol., immunol., cardiovascular, and psychopathol. disorders. For instance, 5-amino-4-(2-chloro-4-methylphenyl)-3-methylpyrazole was cyclized with Et acetoacetate in AcOH to give 42% 7-hydroxy-5-methyl-3-(2-chloro-4-methylphenyl)pyrazolo[1,5-a]pyrimidine. The latter was treated with POCl3 and PhNEt2 to give the 7-chloro analog (84%), which reacted with 3-pentylamine to give 60% title compound III.

Searched by Noble Jarrell

ST azolo triazine pyrimidine prepn CRF antagonist; corticotropin releasing factor antagonist pyrazolopyrimidine pyrazolotriazine prepn antidepressant anxiolytic; azolotriazine azolopyrimidine prepn CRF receptor antagonist

IT Drugs
(gastrointestinal; preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT Intestine, disease
(irritable bowel syndrome, treatment; preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT Anti-inflammatory agents
Antidepressants
Anxiolytics
Cardiovascular agents
Immunomodulators
Nervous system agents
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT Corticotropin releasing factor receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT 1000-84-6P 202578-49-2P 202578-50-5P 202579-55-3P 202579-56-4P
202580-61-8P, 1-Cyano-1-(2,4-dimethylphenyl)propan-2-one
202580-62-9P 202580-64-1P 202580-66-3P 202580-68-5P 202580-69-6P
202580-70-9P 234778-65-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT 9015-71-8, Corticotropin releasing factor
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT 105-53-3, Diethyl malonate 105-58-8 141-78-6, Acetic acid ethyl ester, reactions 141-97-9 616-24-0, 3-Pentylamine 622-79-7, Benzyl azide 1445-45-0, Trimethyl orthoacetate 2208-07-3 34688-71-6, 2,4,6-Trimethylbenzyl cyanide 68429-53-8, 2,4-Dimethylphenylacetonitrile 78531-29-0, 1,3-Dimethoxy-2-aminopropane 202580-72-1 202580-73-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT 202578-52-7P 202578-53-8P 202578-54-9P 202578-55-0P 202578-57-2P
202578-58-3P 202578-59-4P 202578-60-7P 202578-61-8P 202578-62-9P
202578-63-0P 202578-64-1P 202578-65-2P 202578-66-3P 202578-67-4P
202578-68-5P 202578-69-6P 202578-70-9P 202578-71-0P 202578-72-1P
202578-73-2P 202578-74-3P 202578-75-4P 202578-76-5P 202578-77-6P
202578-78-7P 202578-79-8P 202578-80-1P 202578-81-2P 202578-82-3P
202578-83-4P 202578-84-5P 202578-85-6P 202578-86-7P 202578-88-9P
202578-90-3P 202578-92-5P 202578-93-6P 202578-94-7P 202578-95-8P
202578-96-9P 202578-97-0P 202578-98-1P 202578-99-2P 202579-00-8P
202579-01-9P 202579-02-0P 202579-03-1P 202579-04-2P 202579-05-3P
202579-06-4P 202579-08-6P 202579-10-0P 202579-12-2P 202579-14-4P
202579-16-6P 202579-18-8P 202579-20-2P 202579-22-4P 202579-23-5P
202579-25-7P 202579-27-9P 202579-29-1P 202579-30-4P 202579-32-6P
202579-34-8P 202579-36-0P 202579-38-2P 202579-39-3P 202579-41-7P
202579-43-9P 202579-45-1P 202579-46-2P 202579-47-3P 202579-48-4P
202579-49-5P 202579-50-8P 202579-51-9P 202579-52-0P 202579-53-1P
202579-54-2P 202579-57-5P 202579-58-6P 202579-59-7P 202579-60-0P
202579-61-1P 202579-62-2P 202579-63-3P 202579-64-4P 202579-65-5P
202579-66-6P 202579-68-8P 202579-69-9P 202579-70-2P 202579-71-3P
202579-72-4P 202579-73-5P 202579-74-6P 202579-75-7P 202579-76-8P
202579-77-9P 202579-78-0P 202579-79-1P 202579-80-4P 202579-81-5P
202579-82-6P 202579-83-7P 202579-84-8P 202579-85-9P 202579-86-0P
202579-87-1P 202579-88-2P 202579-89-3P 202579-90-6P 202579-91-7P
202579-92-8P 202579-93-9P 202579-94-0P 202579-95-1P 202579-96-2P
202579-97-3P 202579-98-4P 202579-99-5P 202580-00-5P 202580-01-6P
202580-02-7P 202580-03-8P 202580-04-9P 202580-05-0P 202580-06-1P
202580-07-2P 202580-08-3P 202580-09-4P 202580-10-7P 202580-11-8P
202580-12-9P 202580-13-0P 202580-14-1P 202580-15-2P 202580-16-3P
202580-17-4P 202580-18-5P 202580-19-6P 202580-20-9P 202580-21-0P
202580-22-1P 202580-23-2P 202580-24-3P 202580-25-4P 202580-26-5P
202580-27-6P 202580-28-7P 202580-29-8P 202580-31-2P 202580-32-3P
202580-34-5P 202580-35-6P 202580-36-7P 202580-37-8P 202580-39-0P
202580-53-8P 202580-54-9P 202580-56-1P 202580-57-2P 202580-58-3P
202580-59-4P 202580-60-7P 234776-70-6P 234776-71-7P 234776-72-8P
234776-73-9P 234776-74-0P 234776-75-1P 234776-76-2P 234776-77-3P
234776-78-4P 234776-79-5P 234776-80-8P 234776-81-9P 234776-82-0P

234776-83-1P 234776-84-2P 234776-85-3P 234776-86-4P 234776-87-5P
234776-88-6P 234776-89-7P 234776-90-0P 234776-91-1P 234776-92-2P
234776-93-3P 234776-94-4P 234776-95-5P 234776-96-6P 234776-97-7P
234776-98-8P 234776-99-9P 234777-00-5P 234777-01-6P 234777-02-7P
234777-03-8P 234777-04-9P 234777-05-0P 234777-06-1P 234777-07-2P
234777-08-3P 234777-09-4P 234777-10-7P 234777-11-8P 234777-12-9P
234777-13-0P 234777-14-1P 234777-15-2P 234777-16-3P 234777-17-4P
234777-18-5P 234777-19-6P 234777-20-9P 234777-21-0P 234777-22-1P
234777-23-2P 234777-24-3P 234777-25-4P 234777-26-5P 234777-27-6P
234777-28-7P 234777-29-8P 234777-30-1P 234777-31-2P 234777-32-3P
234777-33-4P 234777-34-5P 234777-35-6P 234777-36-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compound; preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT 234777-37-8P 234777-38-9P 234777-39-0P 234777-40-3P 234777-42-5P
234777-43-6P 234777-44-7P 234777-45-8P 234777-46-9P 234777-47-0P
234777-48-1P 234777-49-2P 234777-50-5P 234777-51-6P 234777-52-7P
234777-53-8P 234777-54-9P 234777-55-0P 234777-56-1P 234777-57-2P
234777-58-3P 234777-59-4P 234777-60-7P 234777-61-8P 234777-62-9P
234777-63-0P 234777-64-1P 234777-65-2P 234777-66-3P 234777-67-4P
234777-68-5P 234777-69-6P 234777-70-9P 234777-71-0P 234777-72-1P
234777-73-2P 234777-74-3P 234777-75-4P 234777-76-5P 234777-77-6P
234777-78-7P 234777-79-8P 234777-80-1P 234777-81-2P 234777-82-3P
234777-83-4P 234777-84-5P 234777-85-6P 234777-86-7P 234777-87-8P
234777-88-9P 234777-89-0P 234777-90-3P 234777-91-4P 234777-92-5P
234777-93-6P 234777-94-7P 234777-95-8P 234777-96-9P 234777-97-0P
234777-98-1P 234777-99-2P 234778-00-8P 234778-01-9P 234778-02-0P
234778-03-1P 234778-04-2P 234778-05-3P 234778-06-4P 234778-07-5P
234778-08-6P 234778-09-7P 234778-10-0P 234778-11-1P 234778-12-2P
234778-13-3P 234778-14-4P 234778-15-5P 234778-16-6P 234778-17-7P
234778-18-8P 234778-19-9P 234778-20-2P 234778-21-3P 234778-22-4P
234778-23-5P 234778-24-6P 234778-25-7P 234778-26-8P 234778-27-9P
234778-28-0P 234778-29-1P 234778-30-4P 234778-31-5P 234778-32-6P
234778-33-7P 234778-34-8P 234778-35-9P 234778-36-0P 234778-37-1P
234778-38-2P 234778-39-3P 234778-40-6P 234778-41-7P 234778-42-8P
234778-43-9P 234778-44-0P 234778-45-1P 234778-46-2P 234778-47-3P
234778-48-4P 234778-49-5P 234778-50-8P 234778-51-9P 234778-52-0P
235083-80-4P 261966-75-0P 262297-98-3P 267233-42-1P 267233-43-2P
267233-44-3P 267233-45-4P 267233-46-5P 267233-47-6P 267233-48-7P
267233-49-8P 267233-50-1P 267233-51-2P 267233-52-3P 267233-53-4P
267233-54-5P 267233-55-6P 267233-56-7P 267233-57-8P 267233-59-0P
267233-60-3P 267233-61-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compound; preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

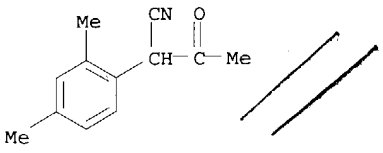
RE.CNT 68 THERE ARE 68 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Anon; JP 4211753 1967
(2) Anon; JP 6157587 1986
(3) Anon; EP 0269859 1988 HCAPLUS
(4) Anon; EP 0300688 1989 HCAPLUS
(5) Anon; EP 0373891 1989 HCAPLUS
(6) Anon; EP 0374448 1990 HCAPLUS
(7) Anon; EP 0395144 1990 HCAPLUS
(8) Anon; EP 0455545 1991 HCAPLUS
(9) Anon; EP 0503099 1992 HCAPLUS
(10) Anon; DE 4243279 1992 HCAPLUS
(11) Anon; WO 9210098 1992 HCAPLUS
(12) Anon; WO 9220642 1992 HCAPLUS
(13) Anon; EP 0521622 1993 HCAPLUS
(14) Anon; EP 0531901 1993 HCAPLUS
(15) Anon; EP 0576350 1993 HCAPLUS
(16) Anon; EP 0591528 1994 HCAPLUS
(17) Anon; EP 0594149 1994 HCAPLUS
(18) Anon; WO 9409017 1994 HCAPLUS
(19) Anon; WO 9413643 1994 HCAPLUS
(20) Anon; WO 9413644 1994 HCAPLUS
(21) Anon; WO 9413661 1994 HCAPLUS
(22) Anon; WO 9413676 1994 HCAPLUS
(23) Anon; WO 9413677 1994 HCAPLUS
(24) Anon; EP 0662477 1995 HCAPLUS
(25) Anon; EP 0714898 1995 HCAPLUS

(26) Anon; WO 9500507 1995 HCAPLUS
(27) Anon; WO 9511880 1995 HCAPLUS
(28) Anon; WO 9532710 1995 HCAPLUS
(29) Anon; WO 9533727 1995 HCAPLUS
(30) Anon; WO 9533750 1995 HCAPLUS
(31) Anon; WO 9534563 1995 HCAPLUS
(32) Anon; EP 0729758 1996 HCAPLUS
(33) Anon; WO 9535298 1996 HCAPLUS
(34) Anon; WO 9619452 1996 HCAPLUS
(35) Anon; WO 9623783 1996 HCAPLUS
(36) Anon; WO 9635689 1996 HCAPLUS
(37) Anon; WO 9639388 1996 HCAPLUS
(38) Anon; WO 9639400 1996 HCAPLUS
(39) Anon; EP 0773023 1997 HCAPLUS
(40) Anon; EP 0778277 1997 HCAPLUS
(41) Anon; EP 0812831 1997 HCAPLUS
(42) Anon; WO 9700868 1997 HCAPLUS
(43) Anon; WO 9714684 1997 HCAPLUS
(44) Anon; WO 9729109 1997 HCAPLUS
(45) Anon; WO 9729110 1997 HCAPLUS
(46) Anon; WO 9808821 1998 HCAPLUS
(47) Anon; WO 9808846 1998 HCAPLUS
(48) Anon; WO 9808847 1998 HCAPLUS
(49) Bantick; US 5428044 1995 HCAPLUS
(50) Barker; US 5089499 1992 HCAPLUS
(51) Britton; Life Sciences 1982, V31, P363 HCAPLUS
(52) Britton; Psychopharmacology 1988, V94, P306 HCAPLUS
(53) Bussler; US 5484760 1996 HCAPLUS
(54) Courtemanche; US 5464847 1995 HCAPLUS
(55) Eicken; US 4567263 1986 HCAPLUS
(56) Hashimoto; US 5137887 1992 HCAPLUS
(57) Himmelsbach; US 5463071 1995 HCAPLUS
(58) Himmler; US 4909647 1991
(59) Kruger; US 4892576 1990 HCAPLUS
(60) Nugent; US 5397774 1995 HCAPLUS
(61) O'Brien; US 3910907 1975 HCAPLUS
(62) Rooney; US 3995039 1976 HCAPLUS
(63) Schonafinger; US 5486531 1996 HCAPLUS
(64) Springer; US 3920652 1975 HCAPLUS
(65) Springer; US 4021556 1977 HCAPLUS
(66) Vinogradoff; US 4997940 1991 HCAPLUS
(67) Weinheim; Arch Pharm 1987, V320, P487
(68) Yuan; US 5723608 1998 HCAPLUS

IT **202580-61-8P**, 1-Cyano-1-(2,4-dimethylphenyl)propan-2-one
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

RN 202580-61-8 HCAPLUS

CN Benzeneacetonitrile, .alpha.-acetyl-2,4-dimethyl- (9CI) (CA INDEX NAME)



L22 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2000:125866 HCAPLUS

DN 132:231516

ED Entered STN: 24 Feb 2000

TI The discovery of 4-(3-pentylamino)-2,7-dimethyl-8-(2-methyl-4-methoxyphenyl)-pyrazolo-[1,5-a]-pyrimidine: a corticotropin-releasing factor (hCRF1) antagonist

AU Gilligan, Paul J.; Baldauf, Caryn; Cocuzza, Anthony; Chidester, Dennis; Zaczek, Robert; Fitzgerald, Lawrence W.; McElroy, John; Smith, Mark A.; Shen, H.-S. L.; Saye, Jo Anne; Christ, David; Trainor, George; Robertson, David W.; Hartig, Paul

CS Chemical and Physical Sciences Department, Experimental Station, **DuPont** Pharmaceuticals Co., Wilmington, DE, 10880-0500, USA

SO Bioorganic & Medicinal Chemistry (2000), 8(1), 181-189
CODEN: BMECEP; ISSN: 0968-0896

PB Elsevier Science Ltd.
DT Journal
LA English
CC 1-3 (Pharmacology)
Section cross-reference(s): 28
AB Structure-activity relationship studies led to the discovery of 4-(3-pentylamino)-2,7-dimethyl-8-(2-methyl-4-methoxyphenyl)-pyrazolo-[1,5-a]-pyrimidine (compound 11-31, DMP904), whose pharmacol. profile strongly supports the hypothesis that hCRF1 antagonists may be potent anxiolytic drugs. Compound 11-31 (hCRF1 Ki = 1.0 .+-. 0.2 nM (n = 8)) was a potent antagonist of hCRF1-coupled adenylate cyclase activity in HEK293 cells (IC50 = 10.0 .+-. 0.01 nM vs. 10 nM r/hCRF, n = 8); .alpha.-helical CRF(9-41) had weaker potency (IC50 = 286 .+-. 63 nM, n = 3). Analog 11-31 had good oral activity in the rat situational anxiety test; the min. ED for 11-31 was 0.3 mg/kg, orally. Maximal efficacy (approx. 57% reduction in latency time in the dark compartment) was observed at this dose. Chlordiazepoxide caused a 72% reduction in latency at 20 mg/kg, orally. CP154526-1 (30 mg/kg, orally) was inactive in this test. Compound 11-31 did not inhibit open-field locomotor activity at 10, 30, and 100 mg/kg, orally in rats. In beagle dogs, this compound (5 mg/kg, i.v., orally) afforded good plasma levels. The key i.v. pharmacokinetic parameters were t1/2, CL and Vd.ss values equal to 46.4 .+-. 7.6 h, 0.49 .+-. 0.08 L/kg/h and 23.0 .+-. 4.2 L/kg, resp. After oral dosing, the mean Cmax, Tmax, t1/2 and bioavailability values were equal to 1260 .+-. 290 nM, 0.75 .+-. 0.25 h, 45.1 .+-. 10.2 h and 33.1%, resp. The overall rat behavioral profile of this compound suggests that it may be an anxiolytic drug with a low motor side effect liability.
ST pyrazolopyrimidine prepn structure CRF1 receptor antagonist; corticotropin releasing factor antagonist pyrazolopyrimidine; DMP904 anxiolytic CRF1 receptor antagonist
IT Structure-activity relationship
(receptor-binding; structure-activity relationships of pyrazolo-[1,5-a]-pyrimidines as human CRF1 antagonists leading to discovery of anxiolytic DMP904)
IT Anxiolytics
(structure-activity relationships of pyrazolo-[1,5-a]-pyrimidines as human CRF1 antagonists leading to discovery of anxiolytic DMP904)
IT Corticotropin releasing factor receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(type I; structure-activity relationships of pyrazolo-[1,5-a]-pyrimidines as human CRF1 antagonists leading to discovery of anxiolytic DMP904)
IT 9012-42-4, Adenylate cyclase
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(anxyolitic DMP904 is antagonist of hCRF1-coupled adenylate cyclase activity in HEK293 cells)
IT 202579-74-6P
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(structure-activity relationships of pyrazolo-[1,5-a]-pyrimidines as human CRF1 antagonists leading to discovery of anxiolytic DMP904)
IT 195055-41-5 202579-58-6 202579-60-0 202579-61-1 202579-62-2
202579-63-3 202579-75-7 202579-85-9 202579-86-0 202579-89-3
202579-91-7 202579-93-9 202579-94-0 202579-95-1 202579-96-2
202580-25-4 202580-27-6 202580-28-7 262297-99-4 262298-00-0
262298-01-1
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(structure-activity relationships of pyrazolo-[1,5-a]-pyrimidines as human CRF1 antagonists leading to discovery of anxiolytic DMP904)
IT 202579-57-5P 202579-59-7P 202579-64-4P 202579-65-5P 202579-66-6P
202579-68-8P 202579-69-9P 202579-70-2P 202579-71-3P 202579-72-4P
202579-73-5P 202579-79-1P 202579-80-4P 202579-81-5P 202579-82-6P
202579-83-7P 202579-88-2P 202579-90-6P 202579-92-8P 202580-29-8P
262297-98-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(structure-activity relationships of pyrazolo-[1,5-a]-pyrimidines as human CRF1 antagonists leading to discovery of anxiolytic DMP904)
IT 616-24-0, 3-Pentylamine 52289-56-2
RL: RCT (Reactant); RACT (Reactant or reagent)

(structure-activity relationships of pyrazolo-[1,5-a]-pyrimidines as human CRF1 antagonists leading to discovery of anxiolytic DMP904)

IT **246023-58-5P** 262298-02-2P 262298-03-3P 262298-04-4P 262298-05-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(structure-activity relationships of pyrazolo-[1,5-a]-pyrimidines as human CRF1 antagonists leading to discovery of anxiolytic DMP904)

RE.CNT 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD

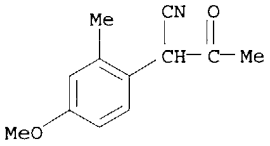
RE

(1) Anon; personal communication from Fitzgerald L W; Smith M A; Baldauf C; He L; Gilligan P; Hartig P; Zaczek R
(2) Anon; personal communication from McElroy J
(3) Anon; personal communication from Saye J A
(4) Anon; personal communication from Shen H L
(5) Anon; personal communication from Smith M A
(6) Anon; private communication from Eyermann J
(7) Arato, M; Biol Psychiatry 1989, V25, P355 MEDLINE
(8) Arvanitis, A; J Med Chem 1999, V42, P808
(9) Banki, C; Am J Psychiatry 1987, V144, P873 MEDLINE
(10) Battaglia, G; Synapse 1987, V1, P572 HCAPLUS
(11) Berridge, C; Brain Res Rev 1990, V15, P71
(12) Chen, C; International Publication Number WO9729109 1997
(13) Chen, Y; J Med Chem 1997, V40, P1749 HCAPLUS
(14) Chorvat, R; J Med Chem 1999, V42, P833 HCAPLUS
(15) Chrousos, G; New Engl J Med 1995, V332, P1351 MEDLINE
(16) Courtmanche, G; US 5464847 1995 HCAPLUS
(17) DeSouza, E; Psychopharmacology: The Fourth Generation of Progress 1995, P505
(18) De Souza, E; J Neurosci 1985, V5, P3189 HCAPLUS
(19) File, S; Neuropharmacology 1987, V26, P877 HCAPLUS
(20) File, S; Stress Med 1988, V4, P221
(21) France, R; Biol Psychiatry 1988, V23, P86 MEDLINE
(22) Ghera, E; Synthesis 1984, P504 HCAPLUS
(23) Gilligan, P; American Chemical Society National Meeting 1998
(24) Gilligan, P; Annual Reports in Medicinal Chemistry 1997, V32, P41 HCAPLUS
(25) Gold, P; Am J Psychiatry 1984, V141, P619 HCAPLUS
(26) Gold, P; New Eng J Med 1986, V314, P1329 MEDLINE
(27) Griebel, G; Psychopharmacology 1998, V138, P55 HCAPLUS
(28) Hodge, C; J Med Chem 1999, V42, P819 HCAPLUS
(29) Holsboer, F; Psychoneuroendocrinology 1984, V9, P147 HCAPLUS
(30) Koob, G; Corticotropin Releasing-factor, Ciba Foundation Symposium 1993, V172, P277 HCAPLUS
(31) Kostich, W; Mol Endocrinology 1998, V12, P1077 HCAPLUS
(32) Mansbach, R; Eur J Pharmacol 1997, V322, P21
(33) Owens, M; Corticotropin-releasing Factor, Ciba Foundation Symposium 1993, V172, P296 HCAPLUS
(34) Perrin, D; Purification of Laboratory Chemicals; 3rd ed 1988
(35) Raadsheer, F; Neuroendocrinology 1994, V60, P436 MEDLINE
(36) Rivier, J; Proc Natl Acad Sci USA 1983, V80, P4851 HCAPLUS
(37) Sapolsky, R; Arch Gen Psychiatry 1989, V46, P1047 MEDLINE
(38) Sawchenko, P; Corticotropin-releasing Factor: Basic and Clinical Studies of a Neuropeptide 1990, P29
(39) Schulz, D; Proc Natl Acad Sci USA 1996, V93, P10477 HCAPLUS
(40) Takahashi, L; Behav Neurosci 1989, V103, P648 MEDLINE
(41) Vale, W; Science 1981, V213, P1394 HCAPLUS
(42) Webster, E; Ann NY Acad Sci 1998, V840, P21 HCAPLUS
(43) Wustrow, D; Bioorg Med Chem Lett 1998, V8, P2067 HCAPLUS

IT **246023-58-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(structure-activity relationships of pyrazolo-[1,5-a]-pyrimidines as human CRF1 antagonists leading to discovery of anxiolytic DMP904)

RN 246023-58-5 HCAPLUS

CN Benzeneacetonitrile, .alpha.-acetyl-4-methoxy-2-methyl- (9CI) (CA INDEX NAME)

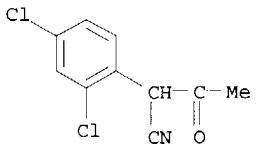


L22 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:60209 HCAPLUS
DN 132:231502
ED Entered STN: 26 Jan 2000
TI 4-(1,3-Dimethoxyprop-2-ylamino)-2,7-dimethyl-8-(2,4-dichlorophenyl)pyrazolo[1,5-a]-1,3,5-triazine: A Potent, Orally Bioavailable CRF1 Receptor Antagonist
AU He, Liqi; Gilligan, Paul J.; Zaczek, Robert; Fitzgerald, Lawrence W.; McElroy, John; Shen, H-S. L.; Saye, Jo Anne; Kalin, Ned H.; Shelton, Steven; Christ, David; Trainor, George; Hartig, Paul
CS Chemical and Physical Sciences Department, **DuPont** Pharmaceuticals Company, Wilmington, DE, 10880-0500, USA
SO Journal of Medicinal Chemistry (2000), 43(3), 449-456
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
CC 1-3 (Pharmacology)
Section cross-reference(s): 28
AB Structure-activity studies in the pyrazolo[1,5-a]-1,3,5-triazine series led to the discovery that compound DMP696 (I) is a potent hCRF1 receptor antagonist (Ki = 1.7 nM vs. 7.5 nM for .alpha.-hel-CRF(9-41), hCRF1 adenylate cyclase IC50 = 82 nM vs. 286 nM for .alpha.-hel-CRF(9-41)). Compound I has excellent oral pharmacokinetic profiles in rats and dogs (37% and 50% oral bioavailabilities, resp.). This compound displays good activity in the rat situational anxiety model (MED = 3 mg/kg orally), whereas a literature standard CP154526-1 was inactive (MED > 30 mg/kg orally). Analog I reduced stereotypical mouth movements in rhesus monkeys by 50% at 21 mg/kg orally using the human intruder paradigm. Overall, the profile of pyrazolotriazine I indicates that hCRF1 receptor antagonists may be anxiolytic agents, which have reduced motor side effect profiles.
ST pyrazolotriazine prepn structure CRF1 receptor anxiolytic; corticotropin releasing factor receptor antagonist pyrazolotriazine
IT Anxiolytics
Drug bioavailability
(preparation of pyrazolotriazine DMP696 as orally bioavailable CRF1 receptor antagonist with anxiolytic activity)
IT Structure-activity relationship
(receptor-binding; CRF1 receptor binding of pyrazolotriazines as potential anxiolytics)
IT Corticotropin releasing factor receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(type I; CRF1 receptor binding of pyrazolotriazines as potential anxiolytics)
IT 202578-53-8 202578-54-9 202578-55-0 202578-57-2 202578-58-3
202578-59-4 202578-60-7 202578-61-8 202578-62-9 202578-63-0
202578-64-1 261966-75-0
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(CRF1 receptor binding of pyrazolotriazines as potential anxiolytics)
IT 202578-52-7P, DMP 696
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolotriazine DMP696 as orally bioavailable CRF1 receptor antagonist with anxiolytic activity)
IT 6306-60-1, 2,4-Dichlorophenylacetonitrile 78531-29-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrazolotriazine DMP696 as orally bioavailable CRF1 receptor antagonist with anxiolytic activity)
IT **76562-15-7P** 202580-70-9P 214416-40-7P 261966-73-8P
261966-74-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrazolotriazine DMP696 as orally bioavailable CRF1 receptor antagonist with anxiolytic activity)
RE.CNT 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Arato, M; Biol Psychiatry 1989, V25, P355 MEDLINE
(2) Arvanitis, A; J Med Chem 1999, V42, P808
(3) Banki, C; Am J Psychiatry 1987, V144, P873 MEDLINE
(4) Battaglia, G; Synapse 1987, V1, P572 HCAPLUS
(5) Berridge, C; Brain Res Rev 1990, V15, P71
(6) Berridge, C; Horm Behav 1987, V21, P393 HCAPLUS

(7) Berridge, C; Regul Pept 1986, V16, P83 HCAPLUS
(8) Britton, D; Life Sci 1982, V31, P363 HCAPLUS
(9) Britton, K; Psychopharmacology 1985, V86, P170 HCAPLUS
(10) Britton, K; Psychopharmacology 1988, V94, P306 HCAPLUS
(11) Chen, Y; J Med Chem 1997, V40, P1749 HCAPLUS
(12) Chorvat, R; J Med Chem 1999, V42, P833 HCAPLUS
(13) Chrousos, G; N Engl J Med 1995, V332, P1351 MEDLINE
(14) Courtmanche, G; US 5464847 1995 HCAPLUS
(15) de Souza, E; J Neurosci 1985, V5, P3189 HCAPLUS
(16) Desouza, E; Corticotropin-releasing factor:basic and clinical studies of a neuropeptide 1990, P335
(17) Desouza, E; Psychopharmacology; The Fourth Generation of Progress 1995, P505
(18) France, R; Biol Psychiatry 1988, V23, P86 MEDLINE
(19) Gilligan, P; Annual Reports in Medicinal Chemistry 1997, V32, P41 HCAPLUS
(20) Gold, P; Am J Psychiatry 1984, V141, P619 HCAPLUS
(21) Gold, P; N Engl J Med 1986, V314, P1329 MEDLINE
(22) Griebel, G; Psychopharmacology 1998, V138, P55 HCAPLUS
(23) Guanowsky, V; Soc Neurosci Abstr 1997, V23, P203.7
(24) He, L; American Chemical Society National Meeting, Abstr MEDI 107 1999
(25) He, L; American Chemical Society National Meeting, Abstr MEDI 4 1999
(26) Hodge, C; J Med Chem 1999, V42, P819 HCAPLUS
(27) Holsboer, F; Psychoneuroendocrinology 1984, V9, P147 HCAPLUS
(28) Kalin, N; Life Sci 1991, V49, P2031 HCAPLUS
(29) Koob, G; Corticotropin-releasing factor, Ciba Foundation Symposium 172 1993, P277 HCAPLUS
(30) Kostich, W; Mol Endocrinol 1998, V12, P1077 HCAPLUS
(31) Mansbach, R; Eur J Pharmacol 1997, V323, P21 HCAPLUS
(32) Owens, M; Corticotropin-releasing factor, Ciba Foundation Symposium 172 1993, P296 HCAPLUS
(33) Perrin, D; Purification of Laboratory Chemicals 3rd ed 1988
(34) Raadsheer, F; Neuroendocrinology 1994, V60, P436 MEDLINE
(35) Rivier, J; Proc Natl Acad Sci U S A 1983, V80, P4851 HCAPLUS
(36) Sapolsky, R; Arch Gen Psychiatry 1989, V46, P1047 MEDLINE
(37) Sawchenko, P; Corticotropin-releasing factor:basic and clinical studies of a neuropeptide 1990, P29
(38) Schulz, D; Proc Natl Acad Sci U S A 1996, V93, P10477 HCAPLUS
(39) Swerdlow, N; Psychopharmacology 1986, V88, P147 HCAPLUS
(40) Takahashi, L; Behav Neurosci 1989, V103, P648 MEDLINE
(41) Timpl, P; Nature Genetics 1998, V19, P162 HCAPLUS
(42) Vale, W; Science 1981, V213, P1394 HCAPLUS
(43) Webster, E; Ann N Y Acad Sci 1998, V840, P21 HCAPLUS
(44) Zaczek, R; American Neuroendocrine Society, Neuroendocrine Workshop on Stress, Abstr 6 1998

IT **76562-15-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrazolotriazine DMP696 as orally bioavailable CRF1 receptor antagonist with anxiolytic activity)

RN 76562-15-7 HCAPLUS
CN Benzeneacetonitrile, .alpha.-acetyl-2,4-dichloro- (9CI) (CA INDEX NAME)



L22 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:495296 HCAPLUS
DN 131:144616
ED Entered STN: 10 Aug 1999
TI Preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists
IN He, Liqi; Gilligan, Paul; Chorvat, Robert; Arvanitis, Argyrios Georgios
PA **Du Pont** Pharmaceuticals Company, USA
SO PCT Int. Appl., 245 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D487-04
ICS A61K031-495; C07D487-04; C07D251-00; C07D231-00; C07D487-04;

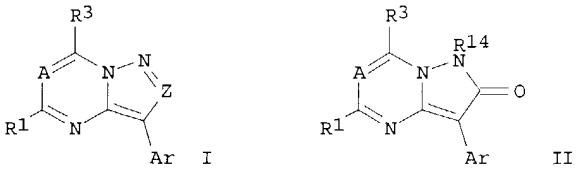
C07D239-00; C07D231-00
CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 2, 63
FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9938868	A1	19990805	WO 1999-US1824	19990128
	W: AU, BR, CA, CN, CZ, EE, HU, IL, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	US 6060478	A	20000509	US 1998-15001	19980128
	US 6191131	B1	20010220	US 1998-15002	19980128
	US 6313124	B1	20011106	US 1998-14734	19980128
	CA 2314613	AA	19990805	CA 1999-2314613	19990128
	AU 9924787	A1	19990816	AU 1999-24787	19990128
	AU 748818	B2	20020613		
	EP 1049699	A1	20001108	EP 1999-904382	19990128
	EP 1049699	B1	20040421		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
	BR 9908206	A	20001205	BR 1999-8206	19990128
	JP 2002501922	T2	20020122	JP 2000-529335	19990128
	NZ 505079	A	20030829	NZ 1999-505079	19990128
	AT 264860	E	20040515	AT 1999-904382	19990128
	ZA 9900843	A	20000802	ZA 1999-843	19990203
PRAI	US 1998-14734	A	19980128		
	US 1998-15001	A	19980128		
	US 1998-15002	A	19980128		
	US 1996-23290P	P	19960724		
	US 1997-899242	A2	19970723		
	WO 1999-US1824	W	19990128		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 9938868	ICM	C07D487-04
	ICS	A61K031-495; C07D487-04; C07D251-00; C07D231-00; C07D487-04; C07D239-00; C07D231-00
US 6060478	ECLA	C07D487/04; C07D487/04; C07D487/04

GI



AB The title compds. [I or II; A = N, CR; Z = N, CR2; Ar = (un)substituted Ph, naphthyl, pyridyl, etc.; R = H, C1-4 alkyl, C2-4 alkenyl, etc.; R1 = H, C1-4 alkyl, C2-4 alkenyl, etc.; R2 = H, C1-4 alkyl, C2-4 alkenyl, etc.; R3 = H, SH, OH, etc.; R14 = C1-10 alkyl, C3-10 alkenyl, C3-10 alkynyl, etc.], corticotropin releasing factor (CRF) antagonists (no data) which are useful in treating anxiety, depression, and other psychiatric, neurol. disorders as well as in treatment of immunol., cardiovascular or heart-related diseases and colonic hypersensitivity associated with psychopathol. disturbance and stress, were prepared and formulated. Thus, treatment of 2,7-dimethyl-8-(2,4-dimethylphenyl)[1,5-a]pyrazolo-1,3,5-triazin-4-one with POCl3 and N,N-dimethylaniline, followed by reaction of the resulting 4-chloro-2,7-dimethyl-8-(2,4-dichlorophenyl)[1,5-a]pyrazolo-1,3,5-triazine with 1,3-dimethoxy-2-aminopropane in EtOH afforded I [A = N; Z = C(Me); R1 = Me; R3 = NHCH(CH2OMe)2; Ar = 2,4-Cl2C6H3].

ST CRF antagonist azolotriazine azolopyrimidine prepn formulation; corticotropin releasing factor antagonist azolotriazine azolopyrimidine prepn; anxiolytic azolotriazine azolopyrimidine prepn formulation; antidepressant azolotriazine azolopyrimidine prepn formulation; hypersensitivity colonic azolotriazine azolopyrimidine prepn formulation; immunol disease azolotriazine azolopyrimidine prepn formulation; cardiovascular agent azolotriazine azolopyrimidine prepn formulation

IT Drugs
(gastrointestinal; preparation of azolotriazines and -pyrimidines as CRF antagonists for treatment of anxiety, depression, and other

psychiatric, neurol. disorders)

IT Intestine, disease
(irritable bowel syndrome; preparation of azolotriazines and -pyrimidines as CRF antagonists for treatment of anxiety, depression, and other psychiatric, neurol. disorders)

IT Anti-inflammatory agents
Antidepressants
Anxiolytics
Cardiovascular agents
Immunomodulators
Nervous system agents
(preparation of azolotriazines and -pyrimidines as CRF antagonists for treatment of anxiety, depression, and other psychiatric, neurol. disorders)

IT Mental disorder
(treatment; preparation of azolotriazines and -pyrimidines as CRF antagonists for treatment of anxiety, depression, and other psychiatric, neurol. disorders)

IT 9015-71-8, Corticotropin-releasing factor
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(antagonists; preparation of azolotriazines and -pyrimidines as CRF antagonists for treatment of anxiety, depression, and other psychiatric, neurol. disorders)

IT **202580-61-8P**, 1-Cyano-1-(2,4-dimethylphenyl)propan-2-one
202580-62-9P 202580-63-0P 202580-64-1P 202580-66-3P 202580-68-5P
202580-70-9P 234778-65-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of azolotriazines and -pyrimidines as CRF antagonists for treatment of anxiety, depression, and other psychiatric, neurol. disorders)

IT 202578-49-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of azolotriazines and -pyrimidines as CRF antagonists for treatment of anxiety, depression, and other psychiatric, neurol. disorders)

IT 202578-50-5P 202578-52-7P 202578-99-2P 202579-08-6P 202579-45-1P
202579-48-4P 202579-49-5P 202579-52-0P 202579-54-2P 202579-55-3P
202579-56-4P 202579-57-5P 202579-86-0P 202580-13-0P 234772-66-8P
234772-67-9P 234772-68-0P 234772-69-1P 234772-70-4P 234772-71-5P
234772-72-6P 234772-73-7P 234772-74-8P 234772-75-9P 234772-76-0P
234772-77-1P 234772-78-2P 234772-79-3P 234772-80-6P 234772-81-7P
234772-82-8P 234772-83-9P 234772-84-0P 234772-85-1P 234772-86-2P
234772-87-3P 234772-88-4P 234772-89-5P 234772-90-8P 234772-91-9P
234772-92-0P 234772-93-1P 234772-94-2P 234772-95-3P 234772-96-4P
234772-97-5P 234772-98-6P 234772-99-7P 234773-00-3P 234773-01-4P
234773-02-5P 234773-03-6P 234773-04-7P 234773-05-8P 234773-07-0P
234773-09-2P 234773-11-6P 234773-13-8P 234773-15-0P 234773-16-1P
234773-18-3P 234773-19-4P 234773-20-7P 234773-21-8P 234773-22-9P
234773-23-0P 234773-24-1P 234773-25-2P 234773-26-3P 234773-27-4P
234773-29-6P 234773-31-0P 234773-33-2P 234773-35-4P 234773-37-6P
234773-38-7P 234773-40-1P 234773-42-3P 234773-44-5P 234773-46-7P
234773-48-9P 234773-50-3P 234773-51-4P 234773-52-5P 234773-53-6P
234773-54-7P 234773-56-9P 234773-58-1P 234773-60-5P 234773-62-7P
234773-64-9P 234773-66-1P 234773-68-3P 234773-70-7P 234773-72-9P
234773-74-1P 234773-75-2P 234773-76-3P 234773-77-4P 234773-78-5P
234773-79-6P 234773-80-9P 234773-81-0P 234773-82-1P 234773-83-2P
234773-84-3P 234773-85-4P 234773-86-5P 234773-87-6P 234773-88-7P
234773-89-8P 234773-90-1P 234773-91-2P 234773-92-3P 234773-93-4P
234773-94-5P 234773-95-6P 234773-96-7P 234773-97-8P 234773-98-9P
234773-99-0P 234774-00-6P 234774-01-7P 234774-02-8P 234774-03-9P
234774-04-0P 234774-05-1P 234774-06-2P 234774-07-3P 234774-08-4P
234774-09-5P 234774-10-8P 234774-11-9P 234774-12-0P 234774-13-1P
234774-14-2P 234774-15-3P 234774-16-4P 234774-17-5P 234774-18-6P
234774-19-7P 234774-20-0P 234774-21-1P 234774-22-2P 234774-23-3P
234774-24-4P 234774-25-5P 234774-26-6P 234774-27-7P 234774-28-8P
234774-29-9P 234774-30-2P 234774-31-3P 234774-32-4P 234774-33-5P
234774-34-6P 234774-35-7P 234774-36-8P 234774-37-9P 234774-38-0P
234774-39-1P 234774-40-4P 234774-41-5P 234774-42-6P 234774-43-7P
234774-44-8P 234774-45-9P 234774-46-0P 234774-47-1P 234774-48-2P
234774-49-3P 234774-50-6P 234774-51-7P 234774-52-8P 234774-53-9P
234774-54-0P 234774-55-1P 234774-57-3P 234774-59-5P 234774-61-9P

234774-63-1P 234774-64-2P 234774-65-3P 234774-66-4P 234774-67-5P
234774-69-7P 234774-74-4P 234774-76-6P 234774-78-8P 234774-80-2P
234774-82-4P 234774-84-6P 234774-86-8P 234774-88-0P 234774-89-1P
234774-91-5P 234774-92-6P 234774-93-7P 234774-94-8P 234774-95-9P
234774-96-0P 234774-97-1P 234774-98-2P 234774-99-3P 234775-00-9P
234775-01-0P 234775-02-1P 234775-03-2P 234775-04-3P 234775-05-4P
234775-06-5P 234775-07-6P 234775-08-7P 234775-09-8P 234775-10-1P
234775-11-2P 234775-12-3P 234775-13-4P 234775-14-5P 234775-15-6P
234775-16-7P 234775-17-8P 234775-18-9P 234775-19-0P 234775-20-3P
234775-21-4P 234775-22-5P 234775-23-6P 234775-24-7P 234775-25-8P
234775-26-9P 234775-27-0P 234775-28-1P 234775-29-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azolotriazines and -pyrimidines as CRF antagonists for treatment of anxiety, depression, and other psychiatric, neurol. disorders)

IT 234775-30-5P 234775-31-6P 234775-32-7P 234775-33-8P 234775-34-9P
234775-35-0P 234775-36-1P 234775-37-2P 234775-38-3P 234775-39-4P
234775-40-7P 234775-41-8P 234775-42-9P 234775-43-0P 234775-44-1P
234775-45-2P 234775-46-3P 234775-47-4P 234775-48-5P 234775-49-6P
234775-50-9P 234775-51-0P 234775-52-1P 234775-53-2P 234775-54-3P
234775-55-4P 234775-56-5P 234775-57-6P 234775-58-7P 234775-59-8P
234775-60-1P 234775-61-2P 234775-62-3P 234775-63-4P 234775-64-5P
234775-65-6P 234775-66-7P 234775-67-8P 234775-68-9P 234775-69-0P
234775-70-3P 234775-71-4P 234775-72-5P 234775-73-6P 234775-74-7P
234775-75-8P 234775-76-9P 234775-77-0P 234775-78-1P 234775-79-2P
234775-80-5P 234775-81-6P 234775-82-7P 234775-83-8P 234775-84-9P
234775-85-0P 234775-86-1P 234775-87-2P 234775-88-3P 234775-89-4P
234775-90-7P 234775-91-8P 234775-92-9P 234775-93-0P 234775-94-1P
234775-95-2P 234775-96-3P 234775-97-4P 234775-98-5P 234775-99-6P
234776-00-2P 234776-01-3P 234776-02-4P 234776-03-5P 234776-04-6P
234776-05-7P 234776-06-8P 234776-07-9P 234776-08-0P 234776-09-1P
234776-10-4P 234776-11-5P 234776-12-6P 234776-13-7P 234776-14-8P
234776-15-9P 234776-16-0P 234776-17-1P 234776-18-2P 234776-19-3P
234776-20-6P 234776-21-7P 234776-22-8P 234776-23-9P 234776-24-0P
234776-25-1P 234776-26-2P 234776-27-3P 234776-28-4P 234776-29-5P
234776-30-8P 234776-31-9P 234776-32-0P 234776-33-1P 234776-34-2P
234776-35-3P 234776-36-4P 234776-37-5P 234776-38-6P 234776-39-7P
234776-40-0P 234776-41-1P 234776-42-2P 234776-43-3P 234776-44-4P
234776-45-5P 234776-46-6P 234776-47-7P 234776-48-8P 234776-49-9P
234776-50-2P 234776-51-3P 234776-52-4P 234776-53-5P 234776-54-6P
234776-55-7P 234776-56-8P 234776-57-9P 234776-58-0P 234776-59-1P
234776-60-4P 234776-61-5P 234776-62-6P 234776-63-7P 234776-64-8P
234776-65-9P 234776-66-0P 234776-67-1P 234776-68-2P 234776-69-3P
234776-70-6P 234776-71-7P 234776-72-8P 234776-73-9P 234776-74-0P
234776-75-1P 234776-76-2P 234776-77-3P 234776-78-4P 234776-79-5P
234776-80-8P 234776-81-9P 234776-82-0P 234776-83-1P 234776-84-2P
234776-85-3P 234776-86-4P 234776-87-5P 234776-88-6P 234776-89-7P
234776-90-0P 234776-91-1P 234776-92-2P 234776-93-3P 234776-94-4P
234776-95-5P 234776-96-6P 234776-97-7P 234776-98-8P 234776-99-9P
234777-00-5P 234777-01-6P 234777-02-7P 234777-03-8P 234777-04-9P
234777-05-0P 234777-06-1P 234777-07-2P 234777-08-3P 234777-09-4P
234777-10-7P 234777-11-8P 234777-12-9P 234777-13-0P 234777-14-1P
234777-15-2P 234777-16-3P 234777-17-4P 234777-18-5P 234777-19-6P
234777-20-9P 234777-21-0P 234777-22-1P 234777-23-2P 234777-24-3P
234777-25-4P 234777-26-5P 234777-27-6P 234777-28-7P 234777-29-8P
234777-30-1P 234777-31-2P 234777-32-3P 234777-33-4P 234777-34-5P
234777-35-6P 234777-36-7P 234777-37-8P 234777-38-9P 234777-39-0P
234777-40-3P 234777-42-5P 234777-43-6P 234777-44-7P 234777-45-8P
234777-46-9P 234777-47-0P 234777-48-1P 234777-49-2P 234777-50-5P
234777-51-6P 234777-52-7P 234777-53-8P 234777-54-9P 234777-55-0P
234777-56-1P 234777-57-2P 234777-58-3P 234777-59-4P 234777-60-7P
234777-61-8P 234777-62-9P 234777-63-0P 234777-64-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azolotriazines and -pyrimidines as CRF antagonists for treatment of anxiety, depression, and other psychiatric, neurol. disorders)

IT 234777-65-2P 234777-66-3P 234777-67-4P 234777-68-5P 234777-69-6P
234777-70-9P 234777-71-0P 234777-72-1P 234777-73-2P 234777-74-3P
234777-75-4P 234777-76-5P 234777-77-6P 234777-78-7P 234777-79-8P
234777-80-1P 234777-81-2P 234777-82-3P 234777-83-4P 234777-84-5P
234777-85-6P 234777-86-7P 234777-87-8P 234777-88-9P 234777-89-0P
234777-90-3P 234777-91-4P 234777-92-5P 234777-93-6P 234777-94-7P

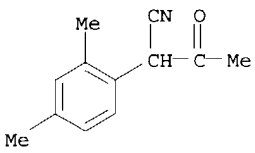
234777-95-8P 234777-96-9P 234777-97-0P 234777-98-1P 234777-99-2P
234778-00-8P 234778-01-9P 234778-02-0P 234778-03-1P 234778-04-2P
234778-05-3P 234778-06-4P 234778-07-5P 234778-08-6P 234778-09-7P
234778-10-0P 234778-11-1P 234778-12-2P 234778-13-3P 234778-14-4P
234778-15-5P 234778-16-6P 234778-17-7P 234778-18-8P 234778-19-9P
234778-20-2P 234778-21-3P 234778-22-4P 234778-23-5P 234778-24-6P
234778-25-7P 234778-26-8P 234778-27-9P 234778-28-0P 234778-29-1P
234778-30-4P 234778-31-5P 234778-32-6P 234778-33-7P 234778-34-8P
234778-35-9P 234778-36-0P 234778-37-1P 234778-38-2P 234778-39-3P
234778-40-6P 234778-41-7P 234778-42-8P 234778-43-9P 234778-44-0P
234778-45-1P 234778-46-2P 234778-47-3P 234778-48-4P 234778-49-5P
234778-50-8P 234778-51-9P 234778-52-0P 234778-53-1P 234778-54-2P
234778-55-3P 234778-56-4P 234778-57-5P 234778-58-6P 234778-59-7P
234778-60-0P 234778-61-1P 234778-62-2P 234778-63-3P 234778-64-4P
235083-80-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azolotriazines and -pyrimidines as CRF antagonists for treatment of anxiety, depression, and other psychiatric, neurol. disorders)

IT 141-97-9, Ethyl acetoacetate 616-24-0, 3-Pentylamine 622-79-7, Benzyl azide 34688-71-6, 2,4,6-Trimethylbenzyl cyanide 68429-53-8, (2,4-Dimethylphenyl)acetonitrile 78531-29-0 202580-72-1 202580-73-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; preparation of azolotriazines and -pyrimidines as CRF antagonists for treatment of anxiety, depression, and other psychiatric, neurol. disorders)

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Chen, Y; WO 9533750 A 1995 HCAPLUS
(2) Du Pont Merck Pharma; WO 9803510 A 1998 HCAPLUS
(3) Janssen Pharmaceutica Nv; WO 9729109 A 1997 HCAPLUS
(4) Jun, Y; WO 9635689 A 1996 HCAPLUS

IT **202580-61-8P**, 1-Cyano-1-(2,4-dimethylphenyl)propan-2-one
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of azolotriazines and -pyrimidines as CRF antagonists for treatment of anxiety, depression, and other psychiatric, neurol. disorders)

RN 202580-61-8 HCAPLUS
CN Benzeneacetonitrile, .alpha.-acetyl-2,4-dimethyl- (9CI) (CA INDEX NAME)



L22 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:87733 HCAPLUS
DN 128:154103
ED Entered STN: 14 Feb 1998
TI Preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists
IN Arvanitis, Argyrios Georgious; Chorvat, Robert John
PA **Du Pont** Merck Pharmaceutical Co., USA
SO PCT Int. Appl., 225 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D487-04
ICS A61K031-505; C07D487-04; C07D239-00; C07D231-00; C07D487-04; C07D251-00; C07D231-00; C07D487-04; C07D249-00; C07D239-00; C07D487-04; C07D251-00; C07D249-00
CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

FAN.CNT 5

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9803510	A1	19980129	WO 1997-US13072	19970723

W: AM, AU, AZ, BR, BY, CA, CN, CZ, EE, HU, IL, JP, KG, KR, KZ, LT,

LV, MD, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, UA, VN, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE

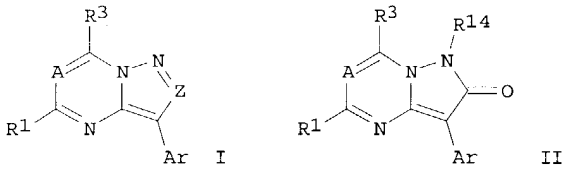
CA	2259583	AA	19980129	CA 1997-2259583	19970723
AU	9738942	A1	19980210	AU 1997-38942	19970723
AU	747708	B2	20020523		
EP	915880	A1	19990519	EP 1997-936222	19970723
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
CN	1225637	A	19990811	CN 1997-196525	19970723
CN	1104432	B	20030402		
BR	9710544	A	19990817	BR 1997-10544	19970723
US	6124289	A	20000926	US 1997-899242	19970723
JP	2002513382	T2	20020508	JP 1998-507233	19970723
ZA	9706603	A	19990125	ZA 1997-6603	19970724
TW	542827	B	20030721	TW 1997-86110640	19970725
LV	12292	B	19991120	LV 1999-13	19990120
NO	9900264	A	19990310	NO 1999-264	19990121
LT	4680	B	20000725	LT 1999-8	19990125
CN	1327793	A	20011226	CN 2001-120849	20010530
AU	773039	B2	20040513	AU 2002-23236	20020312
CN	1388126	A	20030101	CN 2002-118589	20020425
PRAI US	1996-23290P	P	19960724		
US	1996-686047	A	19960724		
US	1997-899242	A	19970723		
AU	1997-38942	A3	19970723		
WO	1997-US13072	W	19970723		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 9803510	ICM	C07D487-04
	ICS	A61K031-505; C07D487-04; C07D239-00; C07D231-00; C07D487-04; C07D251-00; C07D231-00; C07D487-04; C07D249-00; C07D239-00; C07D487-04; C07D251-00; C07D249-00
WO 9803510	ECLA	C07D487/04; C07D487/04; C07D487/04

OS MARPAT 128:154103

GI



AB The title compds. [I or II; A = N, CR; Z = N, CR2; Ar = (un)substituted Ph, naphthyl, pyridyl, etc.; R = H, C1-4 alkyl, C2-4 alkenyl, etc.; R1 = H, C1-4 alkyl, C2-4 alkenyl, etc.; R2 = H, C1-4 alkyl, C2-4 alkenyl, etc.; R3 = H, SH, OH, etc.; R14 = C1-10 alkyl, C3-10 alkenyl, C3-10 alkynyl, etc.], corticotropin releasing factor (CRF) antagonists useful in treating anxiety, depression, and other psychiatric, neurol. disorders as well as in treatment of immunol., cardiovascular or heart-related diseases and colonic hypersensitivity associated with psychopathol. disturbance and stress, were prepared and formulated. Thus, treatment of 2,7-dimethyl-8-(2,4-dimethylphenyl)[1,5-a]pyrazolo-1,3,5-triazin-4-one with POCl3 and N,N-dimethylaniline followed by reaction of the resulting 4-chloro-2,7-dimethyl-8-(2,4-dimethylphenyl)[1,5-a]pyrazolo-1,3,5-triazine with 1,3-dimethoxypropyl-2-aminopropane in EtOH afforded I [A = N; Z = C(Me); R1 = Me; R3 = NHCH(CH2OMe)2; Ar = 2,4-Cl2C6H3].

ST CRF antagonist azolotriazine azolopyrimidine prepn formulation; corticotropin releasing factor azolotriazine azolopyrimidine prepn; anxiolytic azolotriazine azolopyrimidine prepn formulation; antidepressant azolotriazine azolopyrimidine prepn formulation; hypersensitivity colonic azolotriazine azolopyrimidine prepn formulation; immunol disease azolotriazine azolopyrimidine prepn formulation; cardiovascular agent azolotriazine azolopyrimidine prepn formulation

IT Immunity
(disorder, treatment of; preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

IT Allergy
(hypersensitivity, treatment of colonic hypersensitivity associated with psychopathol. disturbance and stress.; preparation of azolotriazines and

-pyrimidines as corticotropin releasing factor (CRF) antagonists)

IT Antidepressants
Anxiolytics
Cardiovascular agents
(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

IT 202578-49-2P 202579-55-3P 202579-56-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

IT 202578-50-5P 202578-51-6P 202578-52-7P 202578-53-8P 202578-54-9P
202578-55-0P 202578-56-1P 202578-57-2P 202578-58-3P 202578-59-4P
202578-60-7P 202578-61-8P 202578-62-9P 202578-63-0P 202578-64-1P
202578-65-2P 202578-66-3P 202578-67-4P 202578-68-5P 202578-69-6P
202578-70-9P 202578-71-0P 202578-72-1P 202578-73-2P 202578-74-3P
202578-75-4P 202578-76-5P 202578-77-6P 202578-78-7P 202578-79-8P
202578-80-1P 202578-81-2P 202578-82-3P 202578-83-4P 202578-84-5P
202578-85-6P 202578-86-7P 202578-88-9P 202578-90-3P 202578-92-5P
202578-93-6P 202578-94-7P 202578-95-8P 202578-96-9P 202578-97-0P
202578-98-1P 202578-99-2P 202579-00-8P 202579-01-9P 202579-02-0P
202579-03-1P 202579-04-2P 202579-05-3P 202579-06-4P 202579-08-6P
202579-10-0P 202579-12-2P 202579-14-4P 202579-16-6P 202579-18-8P
202579-20-2P 202579-22-4P 202579-23-5P 202579-25-7P 202579-27-9P
202579-29-1P 202579-30-4P 202579-32-6P 202579-34-8P 202579-36-0P
202579-38-2P 202579-39-3P 202579-41-7P 202579-43-9P 202579-45-1P
202579-46-2P 202579-47-3P 202579-48-4P 202579-49-5P 202579-50-8P
202579-51-9P 202579-52-0P 202579-53-1P 202579-54-2P 202579-57-5P
202579-58-6P 202579-59-7P 202579-60-0P 202579-61-1P 202579-62-2P
202579-63-3P 202579-64-4P 202579-65-5P 202579-66-6P 202579-67-7P
202579-68-8P 202579-69-9P 202579-70-2P 202579-71-3P 202579-72-4P
202579-73-5P 202579-74-6P 202579-75-7P 202579-76-8P 202579-77-9P
202579-78-0P 202579-79-1P 202579-80-4P 202579-81-5P 202579-82-6P
202579-83-7P 202579-84-8P 202579-85-9P 202579-86-0P 202579-87-1P
202579-88-2P 202579-89-3P 202579-90-6P 202579-91-7P 202579-92-8P
202579-93-9P 202579-94-0P 202579-95-1P 202579-96-2P 202579-97-3P
202579-98-4P 202579-99-5P 202580-00-5P 202580-01-6P 202580-02-7P
202580-03-8P 202580-04-9P 202580-05-0P 202580-06-1P 202580-07-2P
202580-08-3P 202580-09-4P 202580-10-7P 202580-11-8P 202580-12-9P
202580-13-0P 202580-14-1P 202580-15-2P 202580-16-3P 202580-17-4P
202580-18-5P 202580-19-6P 202580-20-9P 202580-21-0P 202580-22-1P
202580-23-2P 202580-24-3P 202580-25-4P 202580-26-5P 202580-27-6P
202580-28-7P 202580-29-8P 202580-30-1P 202580-31-2P 202580-32-3P
202580-33-4P 202580-34-5P 202580-35-6P 202580-36-7P 202580-37-8P
202580-38-9P 202580-39-0P 202580-40-3P 202580-41-4P 202580-42-5P
202580-43-6P 202580-44-7P 202580-46-9P 202580-48-1P 202580-49-2P
202580-50-5P 202580-51-6P 202580-52-7P 202580-53-8P 202580-54-9P
202580-55-0P 202580-56-1P 202580-57-2P 202580-58-3P 202580-59-4P
202580-60-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

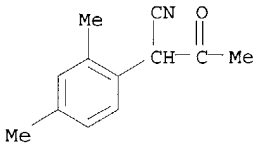
IT 9015-71-8, Corticotropin releasing factor
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)
(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

IT 105-53-3, Diethyl malonate 141-97-9, Ethyl acetoacetate 616-24-0, 3-Pentylamine 622-79-7, Benzyl azide 34688-71-6, 2,4,6-Trimethylbenzyl cyanide 68429-53-8, 2,4-Dimethylphenylacetonitrile 78531-29-0
202580-72-1 202580-74-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

IT **202580-61-8P**, 1-Cyano-1-(2,4-dimethylphenyl)propan-2-one
202580-62-9P 202580-64-1P 202580-65-2P 202580-66-3P 202580-68-5P
202580-69-6P 202580-70-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE
(1) Chen, C; WO 9729109 A 1997 HCAPLUS
(2) Fujisawa Pharmaceutical Co; EP 0531901 A 1993 HCAPLUS
(3) Neurogen Corp; WO 9635689 A 1996 HCAPLUS
(4) Otsuka Pharma Co Ltd; EP 0503099 A 1992 HCAPLUS
(5) Otsuka Pharma Co Ltd; EP 0591528 A 1994 HCAPLUS
(6) Otsuka Pharma Co Ltd; EP 0714898 A 1996 HCAPLUS
(7) Otsuka Seiyaku Kogyo Kk; JP 03204877 A 1991 HCAPLUS
(8) Pfizer; WO 9413676 A 1994 HCAPLUS
(9) Shionogi & Co Ltd; JP 61057587 A 1986 HCAPLUS
(10) Springer, R; US 3920652 A 1975 HCAPLUS
(11) Stanley, R; US 3995039 A 1976 HCAPLUS
(12) Takamizawa; JP 6711753 A HCAPLUS
(13) Takamizawa; JP 6716314 A HCAPLUS
(14) Takamizawa; JP 7030335 A HCAPLUS
IT **202580-61-8P**, 1-Cyano-1-(2,4-dimethylphenyl)propan-2-one
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)
RN 202580-61-8 HCAPLUS
CN Benzeneacetonitrile, .alpha.-acetyl-2,4-dimethyl- (9CI) (CA INDEX NAME)



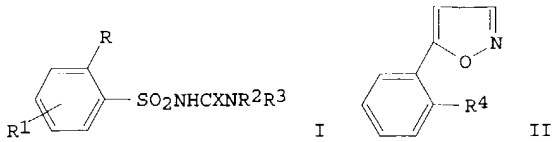
L22 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1983:575812 HCAPLUS
DN 99:175812
ED Entered STN: 12 May 1984
TI Herbicidal sulfonamides
IN Wolf, Anthony David; Rorer, Morris Padgett
PA **du Pont** de Nemours, E. I., and Co. , USA
SO Eur. Pat. Appl., 271 pp.
CODEN: EPXXDW
DT Patent
LA English
IC C07D403-00; C07D417-00; C07D413-00; A01N047-00
CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 5
FAN.CNT 2

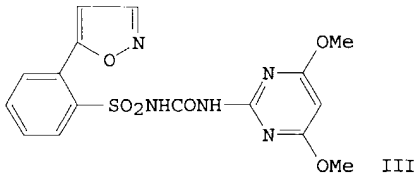
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 83975	A2	19830720	EP 1983-300073	19830106
	EP 83975	A3	19840801		
	EP 83975	B1	19871119		
	R: AT, BE, CH, DE, FR, IT, LI, LU, NL, SE				
	US 4465505	A	19840814	US 1982-428806	19821007
	US 4511392	A	19850416	US 1982-436631	19821029
	AT 30915	E	19871215	AT 1983-300073	19830106
	CA 1239929	A1	19880802	CA 1983-419031	19830106
	US 4606755	A	19860819	US 1984-685026	19841221
	US 4695311	A	19870922	US 1986-861260	19860509
	US 4810282	A	19890307	US 1987-60204	19870610
PRAI	US 1982-337932		19820107		
	US 1982-337934		19820107		
	US 1982-428806		19821007		
	US 1982-436631		19821029		
	EP 1983-300073		19830106		
	US 1984-685026		19841221		
	US 1986-861260		19860509		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
EP 83975	IC	C07D403-00IC C07D417-00IC C07D413-00IC A01N047-00

OS CASREACT 99:175812
GI





AB Benzenesulfonamides I (R = azolyl, azinyl; R1 = H, F, Cl, Br, Me, CF3, OMe; R2 = H, Me; R3 = substituted pyrimidinyl, triazinyl; X = O, S) (67 compds.) were prepared Thus, 2-O2NC6H4COMe was treated with Me2NCH(OMe)2 to give 2-O2NC6H4COCH:CHNMe2, which was cyclized with NH2OH to the isoxazole II (R4 = NO2). Reduction of the nitro group, diazotization, and reaction with SO2-HCl gave II (R4 = SO2Cl), which was amidated and treated with BuNCO and COCl2 to give II (R4 = SO2NCO). Treatment of the isocyanate with 2-amino-4,6-dimethoxypyrimidine gave III which, at 0.05 kg/ha preemergence, gave total control of e.g., nutsedge.

ST benzenesulfonylurea prepn herbicide

IT Herbicides
(benzenesulfonylureas)

IT 19312-06-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(lithiation and reaction of, with sulfur dioxide)

IT 4205-06-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(methylation of)

IT 87488-64-0P **87488-71-9P** 87488-75-3P 87488-81-1P
87488-85-5P 87488-88-8P 87488-93-5P 87488-96-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and amination of)

IT 87488-99-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and chlorination of)

IT 87488-61-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of, with hydroxylamine)

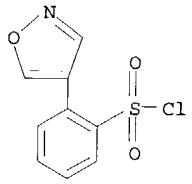
IT 62882-10-4P 87488-63-9P **87488-70-8P** 87488-74-2P
87488-80-0P 87488-92-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and diazotization and reaction of, with sulfur dioxide)

IT 87488-68-4P **87488-73-1P** 87488-77-5P 87488-83-3P
87488-87-7P 87488-90-2P 87488-95-7P 87489-01-8P 87489-02-9P
87489-03-0P 87489-04-1P 87489-05-2P 87489-06-3P 87489-07-4P
87489-08-5P 87489-09-6P 87489-10-9P **87489-11-0P**
87489-12-1P **87489-13-2P** 87489-14-3P 87489-15-4P
87489-16-5P 87489-17-6P 87489-18-7P 87489-19-8P 87489-20-1P
87489-21-2P 87489-22-3P 87489-23-4P 87489-24-5P 87489-25-6P
87489-26-7P 87489-27-8P 87489-28-9P 87489-29-0P 87489-30-3P
87489-31-4P 87489-32-5P 87489-33-6P 87489-34-7P 87489-35-8P
87489-36-9P 87489-37-0P 87489-38-1P 87489-39-2P 87495-41-8P
87495-42-9P **87495-43-0P** **87495-44-1P** 87495-45-2P
87495-46-3P 87495-47-4P 87495-48-5P 87495-49-6P 87495-50-9P
87495-51-0P 87495-52-1P 87495-53-2P 87495-54-3P 87495-55-4P
87509-99-7P 87510-00-7P 87510-01-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and herbicidal activity of)

IT 87488-98-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation and methoxylation of)
IT 87488-65-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with Bu isocyanate)
IT 87488-67-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with aminopyrimidine)
IT 87488-97-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with dichlorotriazine isocyanate)
IT **87488-72-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with dimethoxypyrimidinylcarbamate)
IT 87473-90-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with isoxazoylbenzenesulfonamide)
IT 87488-78-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with methylhydrazine)
IT 87488-66-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with phosgene)
IT 87488-82-2P 87488-86-6P 87488-89-9P 87488-94-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with pyrimidinylcarbamate)
IT 87488-76-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with triazinylcarbamate)
IT 37921-17-8P 87488-62-8P **87488-69-5P** 87488-79-7P
87488-91-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
IT 87489-00-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 5234-26-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with DMF dimethylacetal)
IT 83060-43-9 87473-91-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with benzenesulfonamide)
IT 10564-55-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with benzylthiobenzaldehyde)
IT 75-44-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with butylaminocarbonylbenzenesulfonamide)
IT 614-21-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with dimethoxyformamide dimethylacetal)
IT 53868-36-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with hydroxylamine)
IT 111-36-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with isoxazolylbenzenesulfonamide)
IT 36315-01-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with isoxazolylbenzenesulfonylisocyanate)
IT 4637-24-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with nitroacetophenone)
IT 87488-84-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with sulfuryl chloride)

IT 24852-71-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with tosylmethyl isocyanide)
IT 62882-07-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of)
IT **87488-71-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and amination of)
RN 87488-71-9 HCAPLUS
CN Benzenesulfonyl chloride, 2-(4-isoxazolyl)- (9CI) (CA INDEX NAME)



=> d all fhitstr l28 tot

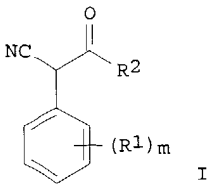
L28 ANSWER 1 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:368618 HCAPLUS
DN 138:368624
ED Entered STN: 14 May 2003
TI Convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles.
IN Zhou, Jiacheng; Oh, Lynette May; Ma, Philip
PA Bristol-Myers Squibb Pharma Company, USA
SO U.S., 20 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC ICM C07D295-033
ICS C07D241-04; C07D211-60; C07D207-06; C07C253-12
NCL 544059000; 558355000; 558309000; 544159000; 544163000; 544399000; 546230000; 548579000
CC 25-20 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
FAN.CNT 2

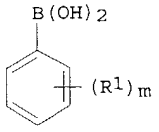
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	US 6562965	B1	20030513	US 2000-610819	20000706	
	US 2003208068	A1	20031106	US 2003-387759	20030313	<--
	US 6727360	B2	20040427			
	US 2004171829	A1	20040902	US 2004-786992	20040225	<--
PRAI	US 1998-80680P	P	19980403	<--		
	US 1999-282508	A3	19990331			
	US 2000-610819	A3	20000706			
	US 2003-387759	A3	20030313			

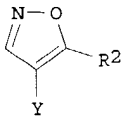
CLASS

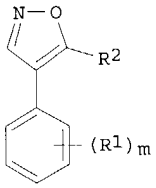
PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES	
US 6562965	ICM	C07D295-033	
	ICS	C07D241-04; C07D211-60; C07D207-06; C07C253-12	
	NCL	544059000; 558355000; 558309000; 544159000; 544163000; 544399000; 546230000; 548579000	
US 6562965	ECLA	C07C255/41	
US 2003208068	ECLA	C07C253/00; C07C255/41; C07D201/08; C07D261/08; C07D261/10B	<--

OS CASREACT 138:368624; MARPAT 138:368624
GI


I


II


III


IV

AB .alpha.-Aryl-.beta.-ketonitriles [I; m = 0-4; R1 = H, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, amino, OH, SH, etc.; R2 = H, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, hydroxyalkyl, haloalkyl, (substituted) alkyl], which serve as synthetic intermediates in the preparation of biol. important mols. such as corticotropin releasing factor (CRF) receptor antagonists, were prepared via reaction of arylboronic acids (II; variables as above) with isoxazoles (III; Y = halo) followed by base treatment of the coupling products (IV; variables as above). Thus, 4-iodo-5-methylisoxazole (preparation given), 2,5-dimethyl-4-methoxybenzeneboronic acid (preparation given), NaHCO3, and [1,1'-bis(diphenylphosphino)ferrocene]palladium dichloride were heated in DME/H2O to give 81.1% 4-(2,5-dimethyl-4-methoxyphenyl)-5-methylisoxazole. The latter was stirred with NaOMe in MeOH to give 92% .alpha.-acetyl-.alpha.-(2,5-dimethyl-4-methoxyphenyl)acetonitrile.

ST arylketonitrile convergent synthesis; nitrile arylketo convergent synthesis

IT Nitriles, preparation
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(oxo; convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)

IT 72287-26-4, [1,1'-Bis(diphenylphosphino)ferrocene]palladium dichloride
RL: CAT (Catalyst use); USES (Uses)
(convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)

IT **246023-57-4P 246023-58-5P**
RL: **IMF (Industrial manufacture)**; **SPN (Synthetic preparation)**; **PREP (Preparation)**
(convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)

IT 1706-11-2, 2,5-Dimethylanisole 5765-44-6, 5-Methylisoxazole 27060-75-9, 4-Bromo-3-methylanisole
RL: RCT (Reactant); RACT (Reactant or reagent)
(convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)

IT 7064-37-1P, 4-Bromo-5-Methylisoxazole 7064-38-2P, 4-Iodo-5-methylisoxazole 58106-25-5P, 4-Bromo-2,5-Dimethylanisole 208399-66-0P, 4-Methoxy-2-methylbenzeneboronic acid 246023-54-1P, 2,5-Dimethyl-4-methoxybenzeneboronic acid **246023-55-2P 246023-56-3P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)

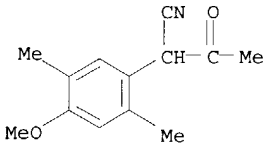
RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) de Munno, A; J Chem Soc, Perkin Trans 2 1977, 9, P1121 HCAPLUS
(2) Dominguez, E; J Org Chem 1966, V61, P5435
(3) Hiroyuki, Y; Chemical Abstracts 1959, V53(22)
(4) Hiroyuki, Y; Yakugaku Zasshi 1959, V79, P623
(5) Labadie, S; Synthetic Communications 1994, V24(5), P709 HCAPLUS
(6) Larock, R; Comprehensive organic transformations 1970, P57
(7) Mitchell, R; J Org Chem 1979, V44, P4733 HCAPLUS
(8) Olah, G; J Org Chem 1993, V58, P3894

(9) Olah, G; Journal of Organic Chemistry 1993, V58, P3194 HCAPLUS
(10) Rouiller, C; Heterocyclic Compounds-More than One Hetero Atom 1962, P3465
(11) Sakakibara, T; Chem Express 1989, V4, P85 HCAPLUS
(12) Sumimoto; US 4797492 A 1989 HCAPLUS
(13) Zhou; US 6107508 A 2000 HCAPLUS

IT **246023-57-4P**
RL: **IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)**
(convergent synthesis of .alpha.-aryl-.beta.-ketonitriles from arylboronic acids and isoxazoles)
RN 246023-57-4 HCAPLUS
CN Benzeneacetonitrile, .alpha.-acetyl-4-methoxy-2,5-dimethyl- (9CI) (CA INDEX NAME)



L28 ANSWER 2 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:965163 HCAPLUS
DN 138:39539
ED Entered STN: 20 Dec 2002
TI Preparation of amino acid derivatives as inhibitors of protein isoprenyl transferases
IN Sebti, Said M.; Hamilton, Andrew D.; Augeri, David J.; Barr, Kenneth J.; Donner, Greg B.; Fakhoury, Stephen A.; O'Connor, Stephen J.; Rosenberg, Saul H.; Shen, Wang; Szczepankiewicz, Bruce G.; Gunawardana, Indrani W.
PA University of Pittsburgh, USA
SO U.S. Pat. Appl. Publ., 499 pp., Cont.-in-part of U.S. Ser. No. 852,858, abandoned.
CODEN: USXXCO
DT **Patent**
LA English
IC ICM C07D045-02
ICS C07D307-56
NCL 544238000; 549321000; 548252000; 544333000; 544405000
CC 34-2 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 7, 28, 63
FAN.CNT 8

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2002193596	A1	20021219	US 2001-984411	20011030 <--
	US 6693123	B2	20040217		
PRAI	US 1995-7247P	P	19951106 <--		
	US 1996-740909	B2	19961105 <--		
	US 1997-852858	B2	19970507 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 2002193596	ICM	C07D045-02
	ICS	C07D307-56
	NCL	544238000; 549321000; 548252000; 544333000; 544405000
US 2002193596	ECLA	C07C237/36; C07D213/70C; C07D213/71; C07D213/71B; C07D213/74E; C07D213/75B2; C07D213/75D3; C07D213/82D; C07D213/82G; C07D213/82H; C07D213/89B; C07D233/54C2D4; C07D233/54C2D2; C07D233/54C2D3; C07D233/54C2D5; C07D233/90; C07D235/06B; C07D237/14; C07D239/26D; C07D239/4B3; C07D241/04; C07D241/12C; C07D241/18; C07D253/06D; C07D257/04D2C1; C07D261/02B; C07D263/2; C07D263/32; C07D265/30C; C07D277/20F1; C07D277/30; C07D277/36; C07D277/48; C07D277/50; C07D295/08B3; C07D295/12B1B1; C07D295/14A3; C07D295/18B1D; C07D295/18B1F; C07D307/54; C07D307/81; C07C239/20; C07D317/30; C07D317/60; C07D333/18; C07D333/20; C07D333/24; C07D040/12; C07D401/12; C07D405/04; C07D405/12; C07D405/12; C07D409/12; C07D417/12; C07D487/08; C07D521/00B1C5; C07D521/00B1N; C07F009/53A7; C07C271/22; C07C317/50; C07C323/59; C07C323/60; C07C327/42; C07D205/04; C07D027/08A; C07D207/09; C07D207/10; C07D207/12; C07D207/26B1;

C07D207/26C; C07D209/48D3A2; C07D021/14; C07D211/42; C07D211/52; C07D211/58; C07D213/30B; C07D213/30C; C07D213/30D2; C07D213/32; C07D213/34; C07D213/36; C07D213/38; C07D213/56; C07D213/64; C07D213/64A; C07D213/65; C07D021/68; C07D213/70B <--

OS MARPAT 138:39539

AB Compds. R3-Z-L1-aryl [aryl is a benzene ring having certain substituents R1, R2, R4; L1 is L4-NR5-L5, L4-O-L5, L4-S(O)m-L5, etc., where L4 and L5 are absent or alk(en)ylene, R5 is H, alkanoyl, alkoxy, alkoxyalkyl, etc.; m = 0-2; Z is a covalent bond, O, S(O)m, an imino group; R3 = (un)substituted pyridyl or imidazolyl; or L1, Z, and R3 together are aminoalkyl, haloalkyl, halo, carboxaldehyde, (carboxaldehyde)alkyl, or hydroxyalkyl (R1 .noteq. H) or L1, Z, R3, and R4 together are an (un)substituted pyrrolidinone ring] were prepared as inhibitors of protein isoprenyl transferases. Thus, N-[4-(3-pyridylcarbonylamino)-2-phenylbenzoyl]methionine hydrochloride, prepared via amidation reaction, showed 93% inhibition of farnesyl transferase at 1x10-5 M.

ST amino acid deriv prepn inhibitor protein isoprenyl transferase

IT Antiarteriosclerotics
(antiatherosclerotics; preparation of amino acid derivs. as inhibitors of protein isoprenyl transferases)

IT Antitumor agents
Atherosclerosis
Neoplasm
(preparation of amino acid derivs. as inhibitors of protein isoprenyl transferases)

IT Amino acids, preparation
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amino acid derivs. as inhibitors of protein isoprenyl transferases)

IT Artery, disease
(restenosis; preparation of amino acid derivs. as inhibitors of protein isoprenyl transferases)

IT 131384-38-8, Protein farnesyltransferase 135371-29-8, Protein geranylgeranyltransferase
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of amino acid derivs. as inhibitors of protein isoprenyl transferases)

IT 645-14-7P, 1H-Imidazole-4-acetaldehyde
RL: BYP (Byproduct); PREP (Preparation)
(preparation of amino acid derivs. as inhibitors of protein isoprenyl transferases)

IT 191100-48-8P 191100-50-2P 191100-75-1P 191101-08-3P 191101-16-3P
191101-26-5P 191101-28-7P 191101-51-6P 191101-63-0P 191101-64-1P
191102-03-1P 191102-18-8P 478907-80-1P 478908-58-6P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of amino acid derivs. as inhibitors of protein isoprenyl transferases)

IT 191100-39-7P 191100-45-5P 191100-74-0P 191100-76-2P 191100-80-8P
191100-82-0P 191100-83-1P 191100-84-2P 191100-86-4P 191100-88-6P
191100-94-4P 191101-01-6P 191101-04-9P 191101-10-7P 191101-11-8P
191101-12-9P 191101-13-0P 191101-14-1P 191101-15-2P 191101-17-4P
191101-19-6P 191101-21-0P 191101-22-1P 191101-23-2P 191101-24-3P
191101-25-4P 191101-27-6P 191101-29-8P 191101-30-1P 191101-31-2P
191101-35-6P 191101-37-8P 191101-40-3P 191101-42-5P 191101-45-8P
191101-47-0P 191101-53-8P 191101-56-1P 191101-58-3P 191101-62-9P
191101-65-2P 191101-66-3P 191101-67-4P 191101-68-5P 191101-69-6P
191101-71-0P 191101-72-1P 191101-73-2P 191101-74-3P 191101-75-4P
191101-76-5P 191101-77-6P 191101-78-7P 191101-80-1P 191101-81-2P
191101-82-3P 191101-83-4P 191101-84-5P 191101-85-6P 191101-86-7P
191101-88-9P 191101-89-0P 191101-90-3P 191101-91-4P 191101-92-5P
191101-93-6P 191101-95-8P 191101-96-9P 191101-97-0P 191101-98-1P
191101-99-2P 191102-00-8P 191102-01-9P 191102-02-0P 191102-04-2P
191102-05-3P 191102-06-4P 191102-07-5P 191102-08-6P 191102-09-7P
191102-10-0P 191102-11-1P 191102-12-2P 191102-13-3P 191102-14-4P
191102-15-5P 191102-16-6P 191102-19-9P 191102-20-2P 191102-23-5P
191102-24-6P 191102-25-7P 191102-26-8P 191102-28-0P 191102-29-1P
191102-30-4P 191102-31-5P 191102-32-6P 191102-33-7P 191102-34-8P
191102-35-9P 191102-36-0P 191102-37-1P 191102-38-2P 191102-39-3P
191102-40-6P 191102-41-7P 191102-43-9P 191102-44-0P 191102-45-1P
191102-46-2P 191102-47-3P 191102-48-4P 191102-49-5P 191102-50-8P
191102-52-0P 191102-53-1P 191102-54-2P 191102-55-3P 191102-56-4P

191102-57-5P 191102-58-6P 191102-59-7P 191102-60-0P 191102-61-1P
191102-62-2P 191102-63-3P 191102-76-8P 191102-78-0P 191102-79-1DP,
1747 191102-79-1P 191102-81-5P 191102-82-6P 191102-83-7P
191102-85-9P 191102-86-0P 191102-88-2P 191104-21-9P 191104-89-9P
191105-25-6P 191105-26-7P 191105-28-9P 191105-30-3P 191105-32-5P
191105-33-6P 215177-73-4P 215919-73-6P 216229-65-1P 216230-18-1P
216232-29-0P 223573-38-4P 225938-38-5P 225938-41-0P 225938-53-4P
225938-58-9P 225938-60-3P 225938-64-7P 225938-75-0P 225938-77-2P
247235-66-1P 247235-67-2P 247235-68-3P 247235-69-4P 247235-72-9P
247235-73-0P 247235-82-1P 251577-09-0P 344900-92-1P 478907-70-9P
478907-71-0P 478907-72-1P 478907-73-2P 478907-74-3P 478907-75-4P
478907-76-5P 478907-77-6P 478907-78-7P 478907-79-8P 478907-81-2P
478907-84-5P 478907-89-0P 478907-90-3P 478907-91-4P 478907-92-5P
478907-93-6P 478907-94-7P 478907-95-8P 478907-96-9P 478907-97-0P
478907-98-1P 478907-99-2P 478908-00-8P 478908-01-9P 478908-02-0P
478908-03-1P 478908-04-2P 478908-05-3P 478908-06-4P 478908-07-5P
478908-08-6P 478908-09-7P 478908-10-0P 478908-11-1P 478908-12-2P
478908-13-3P 478908-14-4P 478908-15-5P 478908-16-6P 478908-17-7P
478908-18-8P 478908-19-9P 478908-20-2P 478908-21-3P 478908-22-4P
478908-23-5P 478908-24-6P 478908-25-7P 478908-26-8P 478908-27-9P
478908-28-0P 478908-29-1P 478908-30-4P 478908-31-5P 478908-32-6P
478908-33-7P 478908-34-8P 478908-35-9P 478908-36-0P 478908-37-1P
478908-38-2P 478908-39-3P **478908-40-6P** 478908-41-7P
478908-42-8P 478908-43-9P
RL: PAC (Pharmacological activity); **SPN (Synthetic preparation)**;
THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**
; USES (Uses)
(preparation of amino acid derivs. as inhibitors of protein isoprenyl transferases)

IT 478908-44-0P 478908-45-1P 478908-46-2P 478908-47-3P 478908-48-4P
478908-49-5P 478908-50-8P 478908-51-9P 478908-52-0P 478908-53-1P
478908-54-2P 478908-55-3P 478908-56-4P 478908-57-5P 478908-59-7P
478908-60-0P 478908-61-1P 478908-62-2P 478909-39-6P 478909-40-9P
478909-41-0P 478909-42-1P 478909-43-2P 478909-44-3P 478909-45-4P
478909-46-5P 478909-47-6P 478909-48-7P 478909-49-8P 478909-50-1P
478909-51-2P 478909-52-3P 478909-53-4P 478909-54-5P 478909-55-6P
478909-73-8P 478909-74-9P 478909-75-0P 478909-76-1P 478909-77-2P
478909-78-3P 478909-79-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amino acid derivs. as inhibitors of protein isoprenyl transferases)

IT 59-67-6, Nicotinic acid, reactions 61-90-5, L-Leucine, reactions
85-46-1, 1-Naphthalenesulfonyl chloride 93-11-8, 2-Naphthalenesulfonyl chloride 96-26-4, 1,3 Dihydroxyacetone 98-10-2, Benzenesulfonamide
98-58-8 98-59-9 98-60-2 98-68-0 98-74-8 98-80-6, Phenylboronic acid 100-55-0, 3-Pyridinemethanol 106-93-4, 1 2 Dibromoethane
108-95-2, Phenol, reactions 109-00-2, 3 Hydroxypyridine 123-62-6, Propionic anhydride 133-59-5, Benzenesulfonyl chloride, 2 methyl
150-13-0, 4 Aminobenzoic acid 288-32-4, Imidazole, reactions 327-57-1, L-Norleucine 349-88-2 372-39-4, 3 5 Difluoroaniline 462-08-8, 3 Aminopyridine 500-22-1, 3 Pyridinecarboxaldehyde 504-24-5, 4 Aminopyridine 504-29-0, 2 Aminopyridine 513-35-9, 2 Methyl 2 butene
536-74-3, Phenylacetylene 556-96-7, 5 Bromo m xylene 590-97-6, Bromomethyl acetate 591-22-0, 3 5 Dimethylpyridine 594-44-5, Ethylsulfonyl chloride 626-61-9 700-38-9, 3 Hydroxy 4 nitrotoluene
777-44-6 872-85-5, 4-Pyridinecarboxaldehyde 917-92-0, tert-Butylacetylene 934-56-5 994-89-8, Ethynyltributyltin 1072-63-5, 1-Vinylimidazole 1120-87-2, 4 Bromopyridine 1122-58-3, 4 Dimethylaminopyridine 1739-84-0, 1 2 Dimethylimidazole 1899-93-0
1939-99-7, Benzylsulfonyl chloride 2185-02-6, L-Homoserine lactone
2208-07-3, Ethyl acetimidate hydrochloride 2315-36-8, 2 Chloro n n diethylacetamide 2486-69-3, 4 Amino 3 methoxybenzoic acid 2486-70-6, 4 Amino 3 methylbenzoic acid 2488-15-5 2491-18-1, L Methionine methyl ester hydrochloride 2537-48-6, Diethyl cyanomethylphosphonate
2666-93-5, L-Leucine methyl ester 2991-42-6 3081-61-6 3081-62-7
3251-69-2, 4 Imidazoleacetic acid hydrochloride 3844-54-0 3900-89-8
4670-56-8 5036-48-6, 1H-Imidazole-1-propanamine 5292-45-5 5337-09-7
5372-81-6 5446-02-6 5720-05-8, 4 Methylphenylboronic acid 5720-06-9, 2 Methoxyphenylboronic acid 5720-07-0, 4 Methoxyphenylboronic acid
5832-44-0 6224-91-5, 1 Trimethylsilyl 1 propyne 6959-48-4, 3 Chloromethylpyridine hydrochloride 7745-93-9, 2 Bromo 4 nitrotoluene
10065-72-2, L-Alanine methyl ester 10111-08-7, 2 Imidazolecarboxaldehyde
10147-37-2, Isopropylsulfonyl chloride 10365-98-7, 3 Methoxyphenylboronic acid 13324-11-3 13922-41-3, 1 Naphthaleneboronic

acid 15084-51-2 15399-22-1 16419-60-6, 2-Methylphenylboronic acid
16420-13-6, Dimethylthiocarbamoyl chloride 16712-69-9 17933-03-8, 3
Methylphenylboronic acid 18997-19-8, Chloromethyl pivalate 20260-53-1,
Nicotinic acid chloride hydrochloride 22840-14-8 25999-04-6,
4-Morpholinesulfonamide 27784-76-5, tert-Butyl diethylphosphonoacetate
29604-19-1 29681-44-5 30925-18-9 31872-62-5, 4-Methoxy 3
nitropyridine 32085-88-4, 3 5 Difluorobenzaldehyde 32673-41-9, 4
Hydroxymethylimidazole hydrochloride 35454-39-8 39555-28-7,
2-Adamantaneethanol 51175-71-4, 3-Thiophenesulfonyl chloride
52536-09-1 53317-09-2 58728-64-6, 4 Amino 1 naphthalenecarbonitrile
67492-50-6 67753-90-6 68559-40-0 74763-88-5 79538-20-8, 3 5
Difluorobenzyl alcohol 90002-36-1 100959-22-6 114081-08-2
136789-15-6 152620-34-3 158063-66-2 165534-79-2 166169-26-2
180977-33-7 191105-36-9 191105-39-2 191105-40-5 191105-41-6
191105-43-8 191105-44-9 191105-46-1 215177-71-2 215919-24-7
302964-21-2 318290-86-7 345964-93-4 478909-57-8 478909-59-0
478909-61-4 478909-62-5 478909-63-6 478909-64-7 478909-67-0
478909-68-1 478909-72-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of amino acid derivs. as inhibitors of protein isoprenyl transferases)

IT 1121-55-7P, 3 Vinylpyridine 2150-47-2P 3430-27-1P 7314-32-1P
13480-38-1P, 4 Nitro 2 phenyltoluene 13511-89-2P 15144-85-1P
16426-64-5P, 2 Bromo 4 nitro benzoic acid 25539-19-9P 31434-93-2P
32018-87-4P, 4 Amino 1 naphthoic acid 33016-47-6P 33769-07-2P
34805-23-7P 38940-67-9P 45533-87-7P, 4 Hydroxymethyl 2 methylimidazole
51990-95-5P 62199-60-4P 66493-39-8P 80715-22-6P 84269-70-5P
84539-35-5P 85391-05-5P 88181-49-1P 92254-03-0P 102676-60-8P
105183-60-6P 106945-71-5P 114077-82-6P 117504-12-8P 118054-54-9P
124391-60-2P, 4 Nitro 2 phenylbenzoic acid 131249-78-0P 133728-31-1P
149543-83-9P 160446-35-5P 160813-66-1P 164362-16-7P 166169-27-3P
166170-19-0P 168169-12-8P 172975-69-8P, 3 5 Dimethylphenylboronic acid
173472-36-1P 179015-63-5P 180863-46-1P 180863-47-2P 180863-61-0P
180976-91-4P 180976-94-7P 180976-95-8P 180976-96-9P 180976-98-1P
180976-99-2P 180977-00-8P 180977-02-0P 180977-03-1P 180977-05-3P
180977-07-5P 180977-08-6P 180977-10-0P 180977-11-1P 180977-38-2P
182499-91-8P 182500-28-3P 185051-42-7P 191101-18-5P 191101-20-9P
191103-39-6P 191103-40-9P 191103-41-0P 191103-42-1P 191103-43-2P
191103-44-3P 191103-46-5P 191103-47-6P 191103-70-5P 191103-71-6P
191103-72-7P 191103-73-8P 191103-74-9P 191103-75-0P 191103-76-1P
191103-77-2P 191103-78-3P 191103-80-7P 191103-85-2P 191103-86-3P
191103-87-4P 191103-88-5P 191103-89-6P 191103-90-9P 191103-91-0P
191103-94-3P 191103-95-4P 191103-96-5P 191103-97-6P 191103-98-7P
191103-99-8P 191104-02-6P 191104-03-7P 191104-04-8P 191104-05-9P
191104-06-0P 191104-07-1P 191104-09-3P 191104-10-6P 191104-15-1P
191104-16-2P 191104-17-3P 191104-18-4P 191104-19-5P 191104-20-8P
191104-22-0P 191104-23-1P 191104-24-2P 191104-25-3P 191104-26-4P
191104-29-7P 191104-30-0P 191104-31-1P 191104-33-3P 191104-34-4P
191104-36-6P 191104-38-8P 191104-41-3P 191104-47-9P 191104-49-1P
191104-50-4P 191104-51-5P 191104-53-7P 191104-57-1P 191104-59-3P
191104-67-3P 191104-69-5P 191104-72-0P 191104-74-2P 191104-78-6P
191104-79-7P 191104-80-0P 191104-81-1P 191104-82-2P 191104-85-5P
191104-87-7P 191104-88-8P 191104-90-2P 191104-92-4P 191104-93-5P
191104-94-6P 191104-95-7P 191104-96-8P 191104-97-9P 191104-98-0P
191104-99-1P 191105-00-7P 191105-01-8P 191105-02-9P 191105-03-0P
191105-04-1P 191105-06-3P 191105-07-4P 191105-09-6P 191105-10-9P
191105-11-0P 191105-12-1P 191105-15-4P 191105-17-6P 191105-18-7P
191105-19-8P 191105-20-1P 191105-22-3P 191105-24-5P 191105-27-8P
191105-31-4P 191105-45-0P 191105-51-8P 191105-54-1P 191171-82-1P
203854-94-8P 215919-30-5P 216228-70-5P 216228-72-7P 216228-75-0P
216228-78-3P 216228-80-7P 216235-25-5P 216237-16-0P 216237-17-1P
216237-87-5P 216768-18-2P 223573-76-0P 223573-95-3P 225920-39-8P
225920-40-1P 225920-47-8P 225920-48-9P 225920-49-0P 225920-51-4P
225920-53-6P 225920-54-7P 244251-52-3P 247236-38-0P 253449-47-7P
478907-56-1P 478907-57-2P 478907-58-3P 478907-59-4P 478907-60-7P
478907-61-8P 478907-62-9P 478907-63-0P 478907-64-1P 478907-65-2P
478907-66-3P 478907-67-4P 478907-68-5P 478907-69-6P 478908-63-3P
478908-64-4P 478908-65-5P 478908-66-6P 478908-67-7P 478908-68-8P
478908-69-9P 478908-70-2P 478908-71-3P 478908-72-4P 478908-73-5P
478908-74-6P 478908-75-7P 478908-76-8P 478908-77-9P 478908-78-0P
478908-79-1P 478908-80-4P 478908-81-5P 478908-82-6P 478908-83-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of amino acid derivs. as inhibitors of protein isoprenyl transferases)

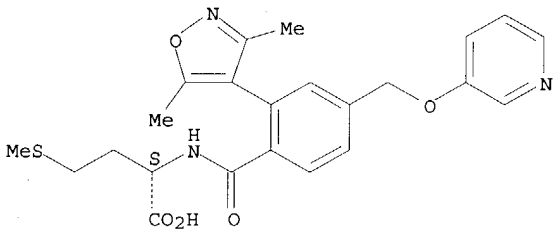
IT 478908-84-8P 478908-85-9P 478908-86-0P 478908-87-1P 478908-88-2P

478908-89-3P 478908-90-6P 478908-91-7P 478908-92-8P 478908-93-9P
478908-94-0P 478908-95-1P 478908-96-2P 478908-97-3P 478908-98-4P
478908-99-5P 478909-00-1P 478909-01-2P 478909-02-3P 478909-03-4P
478909-04-5P 478909-05-6P 478909-06-7P 478909-07-8P 478909-08-9P
478909-09-0P 478909-10-3P 478909-11-4P 478909-12-5P 478909-13-6P
478909-14-7P 478909-15-8P 478909-16-9P 478909-17-0P 478909-18-1P
478909-19-2P 478909-20-5P 478909-21-6P 478909-22-7P 478909-23-8P
478909-24-9P 478909-25-0P 478909-26-1P 478909-27-2P 478909-28-3P
478909-29-4P 478909-30-7P 478909-31-8P 478909-32-9P 478909-33-0P
478909-34-1P 478909-35-2P 478909-36-3P 478909-37-4P 478909-38-5P
478909-56-7P 478909-58-9P 478909-60-3P 478909-65-8P 478909-66-9P
478909-69-2P 478909-70-5P 478909-71-6P 478908-80-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of amino acid derivs. as inhibitors of protein isoprenyl transferases)

IT **478908-40-6P**
RL: PAC (Pharmacological activity); **SPN (Synthetic preparation)**; THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of amino acid derivs. as inhibitors of protein isoprenyl transferases)

RN 478908-40-6 HCAPLUS
CN L-Methionine, N-[2-(3,5-dimethyl-4-isoxazolyl)-4-[(3-pyridinyloxy)methyl]benzoyl]-, monolithium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L28 ANSWER 3 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:369024 HCAPLUS
DN 136:369710
ED Entered STN: 18 May 2002
TI Preparation of heterocyclo substituted hydroxamic acid derivatives as cyclooxygenase-2 and 5-lipoxygenase inhibitors
IN Talley, John J.; Sikorski, James A.; Graneto, Matthew J.; Carter, Jeffery S.; Norman, Bryan H.; Devadas, Balekudru
PA Pharmacia Corp., USA
SO U.S. Pat. Appl. Publ., 54 pp., Cont. of U. S. Ser. No. 624,301.
CODEN: USXXCO
DT **Patent**
LA English
IC ICM C07D043-04
NCL 544238000
CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

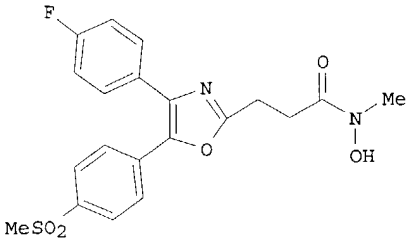
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2002058810	A1	20020516	US 2001-997633	20011129 <--
	US 6696477	B2	20040224		
PRAI	US 1995-450545	A1	19950717 <--		
	US 1997-822528	B1	19970324 <--		
	US 1998-218921	B1	19981222 <--		
	US 2000-624301	A1	20000724		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 20020058810	ICM	C07D043-04
	NCL	544238000

US 2002058810 ECLA B60G017/015C; B64C027/00B; F16F007/10A; F16F015/03 <--
OS MARPAT 136:369710
GI



I

AB Compds. of the formula R2SO2-4-C6H4-A(R1)YR3NR4R5 [A = 5 or 6 membered heterocyclic or carbocyclic ring; Y = alkyl, alkynyl, alkenyl, aryl, aralkyl, cycloalkyl; R1 = heterocyclyl, cycloalkyl, aryl, cycloalkenyl; R2 = alkyl, amino; R3 = bond, CO, (substituted) NHCO, S-CS; R4 = H, OH, alkyl, aryl heterocyclyl, cycloalkyl; R5 = H, alkyl, aryl, heterocyclyl, cycloalkyl] are prepared as antiinflammatory agents. The compds. are useful for treating disorders mediated by cyclooxygenase-2 or 5-lipoxygenase, such as inflammation. Thus, I was prepared from 4-(4-fluorophenyl)-5-(4-(methylsulfonyl)phenyl)-2-oxazolepropionic acid. The IC50 of I was 5.2 .mu.M for COX-2 and 0.05 .mu.M for 5-LO.

ST heterocyclo hydroxamic acid deriv prepn cyclooxygenase inhibitor; lipoxygenase heterocyclo hydroxamic acid deriv prepn inhibitor; antiinflammatory heterocyclo hydroxamic acid deriv prepn

IT Allergy inhibitors
Analgesics
Anti-inflammatory agents
Antiarthritics
Antiasthmatics
(preparation of heterocyclo hydroxamic acid derivs. as cyclooxygenase-2 and 5-lipoxygenase inhibitors)

IT Hydroxamic acids
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclo hydroxamic acid derivs. as cyclooxygenase-2 and 5-lipoxygenase inhibitors)

IT Fever and Hyperthermia
(treatment; preparation of heterocyclo hydroxamic acid derivs. as cyclooxygenase-2 and 5-lipoxygenase inhibitors)

IT 80619-02-9, 5-Lipoxygenase 329900-75-6, Cyclooxygenase-2 329967-85-3, Cyclooxygenase-1
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(inhibitors; preparation of heterocyclo hydroxamic acid derivs. as cyclooxygenase-2 and 5-lipoxygenase inhibitors)

IT 185826-83-9P 185826-85-1P 185826-87-3P 425417-15-8P 425417-17-0P
425417-18-1P 425417-20-5P 425417-22-7P 425417-24-9P 425417-25-0P
425417-27-2P 425417-29-4P 425417-30-7P 425417-33-0P 425417-35-2P
425417-37-4P 425417-39-6P 425417-40-9P 425417-42-1P 425417-44-3P
425417-46-5P 425417-48-7P 425417-50-1P 425417-52-3P 425417-54-5P
425417-56-7P 425417-58-9P 425417-60-3P 425417-62-5P 425417-64-7P
425417-66-9P 425417-68-1P 425417-70-5P 425417-72-7P 425417-74-9P
425417-75-0P **425417-77-2P** **425417-79-4P**
425417-81-8P **425417-83-0P** **425417-85-2P**
425417-87-4P **425417-89-6P** **425417-91-0P**
425417-93-2P 425417-95-4P 425417-97-6P 425417-99-8P
425418-01-5P 425418-03-7P 425418-05-9P 425418-07-1P 425418-09-3P
425418-11-7P 425418-13-9P 425418-15-1P 425418-17-3P 425418-19-5P
425418-21-9P 425418-23-1P 425418-25-3P 425418-26-4P 425418-28-6P
425418-30-0P 425418-32-2P 425418-34-4P 425418-35-5P 425418-36-6P
425418-37-7P 425418-39-9P 425418-41-3P 425418-43-5P 425418-46-8P
425418-48-0P 425418-50-4P 425418-52-6P 425418-54-8P 425418-55-9P
425418-57-1P 425418-59-3P 425418-61-7P 425418-63-9P 425418-65-1P
425418-68-4P 425418-71-9P 425418-74-2P 425418-77-5P 425418-79-7P
425418-81-1P 425418-83-3P 425418-84-4P 425418-85-5P 425418-87-7P
425418-89-9P 425418-91-3P 425418-93-5P 425418-95-7P 425418-97-9P

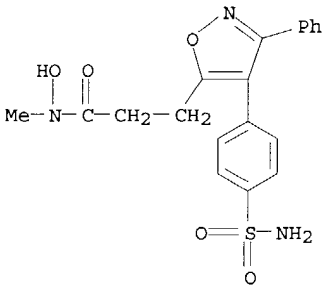
425418-99-1P 425419-01-8P 425419-02-9P 425419-04-1P 425419-06-3P
425419-07-4P 425419-09-6P 425419-11-0P 425419-13-2P 425419-15-4P
425419-17-6P 425419-19-8P 425419-21-2P 425419-22-3P 425419-24-5P
425419-26-7P 425419-28-9P 425419-30-3P 425419-32-5P 425419-34-7P
425419-36-9P 425419-38-1P 425419-39-2P 425419-41-6P
425419-46-1P 425419-48-3P 425419-50-7P
425419-52-9P 425419-54-1P 425419-56-3P
425419-58-5P 425419-60-9P 425419-62-1P
425419-64-3P 425419-66-5P 425419-68-7P 425419-70-1P
425419-72-3P 425419-74-5P 425419-77-8P 425419-80-3P 425419-83-6P
425419-85-8P 425419-87-0P 425419-89-2P 425419-91-6P 425419-93-8P
425419-95-0P **425419-97-2P 425419-98-3P**
425420-00-4P 425420-02-6P 425420-04-8P
425420-06-0P 425420-08-2P 425420-10-6P
425420-12-8P 425420-13-9P 425420-15-1P
425420-17-3P 425420-19-5P 425420-21-9P 425420-23-1P 425420-25-3P
425420-27-5P 425420-29-7P 425420-31-1P 425420-33-3P 425420-35-5P
425420-37-7P 425420-39-9P 425420-41-3P **425420-43-5P**
425420-45-7P 425420-46-8P 425420-48-0P
425420-50-4P 425420-51-5P 425420-53-7P
425420-57-1P 425420-58-2P 425420-60-6P
RL: PAC (Pharmacological activity); **SPN (Synthetic preparation)**; THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)** ; USES (Uses)
(preparation of heterocyclo hydroxamic acid derivs. as cyclooxygenase-2 and 5-lipoxygenase inhibitors)

IT 99-91-2 553-90-2, Dimethyl oxalate 17852-52-7 163303-39-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of heterocyclo hydroxamic acid derivs. as cyclooxygenase-2 and 5-lipoxygenase inhibitors)

IT 39757-35-2P 170570-50-0P 170571-19-4P 170571-20-7P 170571-48-9P
170571-71-8P 185826-92-0P 185826-97-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of heterocyclo hydroxamic acid derivs. as cyclooxygenase-2 and 5-lipoxygenase inhibitors)

IT **425417-77-2P**
RL: PAC (Pharmacological activity); **SPN (Synthetic preparation)**; THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)** ; USES (Uses)
(preparation of heterocyclo hydroxamic acid derivs. as cyclooxygenase-2 and 5-lipoxygenase inhibitors)

RN 425417-77-2 HCAPLUS
CN 5-Isoxazolepropanamide, 4-[4-(aminosulfonyl)phenyl]-N-hydroxy-N-methyl-3-phenyl- (9CI) (CA INDEX NAME)



L28 ANSWER 4 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:84600 HCAPLUS
DN 136:151161
ED Entered STN: 31 Jan 2002
TI Preparation of 4-(heterocyclyl)benzenesulfonamides as components of a combination of a cyclooxygenase-2 inhibitors and a leukotriene B4 receptor antagonist
IN Isakson, Peter C.; Anderson, Gary D.; Gregory, Susan A.
PA G.D. Searle and Co., USA
SO U.S., 19 pp., Cont.-in-part of U.S. Ser. No. 489,415, abandoned.
CODEN: USXXAM
DT **Patent**
LA English

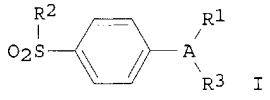
IC ICM A61K031-415
ICS C07D231-02; C07D231-12
NCL 514326000
CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	US 6342510	B1	20020129	US 1996-661641	19960611	<--
	CA 2224563	AA	19961227	CA 1996-2224563	19960611	<--
	US 2002107276	A1	20020808	US 2002-38080	20020103	<--
PRAI	US 1995-489415	B2	19950612	<--		
	US 1996-661641	A1	19960611	<--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES	
US 6342510	ICM	A61K031-415	
	ICS	C07D231-02; C07D231-12	
	NCL	514326000	
US 2002107276	ECLA	A61K045/06	<--

OS MARPAT 136:151161
GI



I

AB The title compds. [I; A = (partially) unsatd. heterocyclyl or carbocyclyl; R1 = (un)substituted heterocyclyl, cycloalkyl, cycloalkenyl, aryl; R2 = Me, NH2; R3 = H, halo, alkyl, etc.] which are cyclooxygenase-2 inhibitors used in combination with a leukotriene B4 receptor antagonists for treatment of inflammation and inflammation-related disorders, were prepared and formulated. Thus, treating Et trifluoroacetate with NaOMe in Me tert-Bu ether followed by addition of 4'-chloroacetophenone (85%), and reacting the resulting 4,4,4-trifluoro-1-(4-chlorophenyl)butane 1,3-dione with 4-sulfonamidophenylhydrazine hydrochloride in EtOH afforded 4-[5-(4-chlorophenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide (80%).
ST heterocyclylbenzenesulfonamide prepn cyclooxygenase COX2 inhibitor combination leukotriene B4; antiarthritic heterocyclylbenzenesulfonamide prepn; antiinflammatory heterocyclylbenzenesulfonamide prepn
IT Leukotriene receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(leukotriene B4; preparation of 4-(1H-pyrazol-1-yl)benzenesulfonamides as antiinflammatories)
IT Anti-inflammatory agents
Antiarthritics
(preparation of 4-(1H-pyrazol-1-yl)benzenesulfonamides as antiinflammatories)
IT 329900-75-6, Cyclooxygenase-2
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of 4-(1H-pyrazol-1-yl)benzenesulfonamides as antiinflammatories)
IT 93014-16-5P, 4-[2-Methyl-4-phenyl-5-oxazolyl]benzenesulfonamide 169590-41-4P, 4-[5-(3-Fluoro-4-methoxyphenyl)-3-(difluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide 169590-42-5P, 4-[5-(4-Methylphenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide 170569-86-5P, 4-[5-(4-Chlorophenyl)-3-(trifluoromethyl)-1H-pyrazol-1-yl]benzenesulfonamide 177660-80-9P, 2-Methyl-5-[1-[4-(methylsulfonyl)phenyl]-4-trifluoromethyl-1H-imidazol-2-yl]pyridine 177660-92-3P, 4-[2-(5-Methylpyridin-3-yl)-4-(trifluoromethyl)-1H-imidazol-1-yl]benzenesulfonamide **181695-72-7P**, 4-[5-Methyl-3-phenylisoxazol-4-yl]benzenesulfonamide 185344-51-8P, 4-[2-Trifluoromethyl-5-(3,4-difluorophenyl)-4-oxazolyl]benzenesulfonamide 185344-55-2P, 4-[2-Trifluoromethyl-5-(3-fluoro-4-methoxyphenyl)-4-oxazolyl]benzenesulfonamide **195061-34-8P**
RL: PAC (Pharmacological activity); **SPN (Synthetic preparation)**; THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of 4-(1H-pyrazol-1-yl)benzenesulfonamides as antiinflammatories)
IT 99-91-2, 4'-Chloroacetophenone 321-28-8, 2-Fluoroanisole 383-63-1,

Ethyl trifluoroacetate 454-31-9, Ethyl difluoroacetate 27918-19-0, 4-Sulfonamidophenylhydrazine hydrochloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 4-(1H-pyrazol-1-yl)benzenesulfonamides as antiinflammatories)

IT 455-91-4P, 3'-Fluoro-4'-methoxyacetophenone 18931-60-7P, 4,4,4-Trifluoro-1-[4-chlorophenyl]butane-1,3-dione 170570-77-1P, 4,4-Difluoro-1-(3-fluoro-4-methoxyphenyl)butane-1,3-dione
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 4-(1H-pyrazol-1-yl)benzenesulfonamides as antiinflammatories)

IT 60940-34-3, Ebselen 71125-38-7, Meloxicam 80937-31-1, Flosulide 110501-66-1, TMK 688 117423-95-7, LY 213024 123653-11-2, Taisho NS 398 128253-31-6, Bay-X 1005 133430-69-0, ETH 615 134578-96-4, ONO 4057 135199-82-5, LY 264086 135893-33-3, PF 10042 136326-31-3, WAY 121006 142422-79-5, RP 66153 146461-98-5, SM 15178 147398-01-4, CGS 25019C 147432-77-7, BI RM 270 150399-22-7, SB 201993 153633-01-3, SC 53228 161172-51-6, LY 293111 162011-90-7, 2(5H)-Furanone, 4-[4-(methylsulfonyl)phenyl]-3-phenyl- 180208-37-1, SB 201146
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of 4-(1H-pyrazol-1-yl)benzenesulfonamides as antiinflammatories)

RE.CNT 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

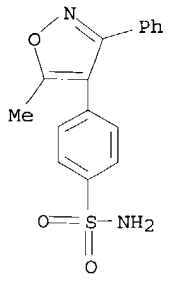
(1) Anon; EP 485111 1992 HCAPLUS
(2) Anon; WO 9404522 1994 HCAPLUS
(3) Anon; WO 9413635 1994 HCAPLUS
(4) Anon; WO 9415932 1994 HCAPLUS
(5) Anon; WO 9420480 1994 HCAPLUS
(6) Anon; WO 9426731 1994 HCAPLUS
(7) Anon; WO 9427980 1994 HCAPLUS
(8) Anon; WO 9500501 1994 HCAPLUS
(9) Anon; DE A4228201 1994
(10) Anon; WO 9603387 1996 HCAPLUS
(11) Anon; WO 9603388 1996 HCAPLUS
(12) Anon; WO 9606840 1996 HCAPLUS
(13) Anon; J Allergy Clinl Immunol 1988, V81, P110
(14) Anon; J Basamajian Spine 1989, V14, P438
(15) Beaver; Am J Med 1984, V77, P38 HCAPLUS
(16) Chang; Acta Pharmacologica Sinica 1991, V12(2), P121 HCAPLUS
(17) Deason; US 4923891 A 1990 HCAPLUS
(18) Dereu; US 5366982 A 1994 HCAPLUS
(19) Djuric; US 4970234 A 1990 HCAPLUS
(20) Djuric; US 5212198 A 1993 HCAPLUS
(21) Djuric; US 5310951 A 1994 HCAPLUS
(22) Djuric; US 5380740 A 1995 HCAPLUS
(23) Ducharme; US 5474995 A 1995 HCAPLUS
(24) Eggler; US 5384318 A 1995 HCAPLUS
(25) Fossaluzza, V; Int J Clin Pharm Res 1992, VXII, P99
(26) Gleason; US 4871771 A 1989 HCAPLUS
(27) Greenwald, R; J Rheumatol 1992, V19, P927 HCAPLUS
(28) Guth; Proc Natl Acad Sci USA 1994, V91, P12308 HCAPLUS
(29) Huang; US 5210208 A 1993 HCAPLUS
(30) Huang; US 5232948 A 1993 HCAPLUS
(31) Hughes; Dermatology 1992, V184, P54 MEDLINE
(32) Isakson; US 5700816 A 1997 HCAPLUS
(33) Konno; US 5256686 A 1993 HCAPLUS
(34) Lau; US 5510368 A 1996 HCAPLUS
(35) Lightman; Am J Ophthalmol 1989, V108, P94
(36) Main; US 5246965 A 1993 HCAPLUS
(37) Mueller; US 5272178 A 1993 HCAPLUS
(38) Musser; US 4889935 A 1989 HCAPLUS
(39) Norman; US 5380738 A 1995 HCAPLUS
(40) Reitz; US 5344991 A 1994 HCAPLUS
(41) Reitz; US 5393790 A 1995 HCAPLUS
(42) Seideman; Acta Orthop Scand 1993, V64, P285 MEDLINE
(43) Seifert; Curr Med Res Opin 1980, V7, P38 MEDLINE
(44) Stewart; Clin Pharmacol Ther 1990, V47, P540 MEDLINE
(45) Talley; US 5434178 A 1995 HCAPLUS
(46) Talley; US 5466823 A 1995 HCAPLUS
(47) Teicher; Cancer Chemother Pharmacol 1994, V33, P515 HCAPLUS
(48) Tennant; J Pharm Pharmacol 1987, V39, P309 HCAPLUS
(49) Tramposch; Inflammation 1993, V17, P531 HCAPLUS
(50) Willikens; Arthritis Rheum 1976, V19, P677

IT **181695-72-7P**, 4-[5-Methyl-3-phenylisoxazol-4-yl]benzenesulfonamide

RL: PAC (Pharmacological activity); **SPN (Synthetic preparation)**; THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)** ; USES (Uses)
(preparation of 4-(1H-pyrazol-1-yl)benzenesulfonamides as antiinflammatories)

RN 181695-72-7 HCAPLUS

CN Benzenesulfonamide, 4-(5-methyl-3-phenyl-4-isoxazolyl)- (9CI) (CA INDEX NAME)



L28 ANSWER 5 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2001:813420 HCAPLUS

DN 135:344507

ED Entered STN: 08 Nov 2001

TI Preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists

IN He, Liqi; Gilligan, Paul; Chorvat, Robert; Arvanitis, Argyrios Georgios

PA Dupont Pharmaceuticals Company, USA

SO U.S., 57 pp., Cont.-in-part of U.S. Ser. No. 899,242.
CODEN: USXXAM

DT **Patent**

LA English

IC A61K031-535; C07D487-04

NCL 514246000

CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 2, 63

FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6313124	B1	20011106	US 1998-14734	19980128 <--
	US 6124289	A	20000926	US 1997-899242	19970723 <--
	ZA 9706603	A	19990125	ZA 1997-6603	19970724 <--
	US 6136809	A	20001024	US 1998-14999	19980128 <--
	LT 4680	B	20000725	LT 1999-8	19990125 <--
	CA 2314613	AA	19990805	CA 1999-2314613	19990128 <--
	WO 9938868	A1	19990805	WO 1999-US1824	19990128 <--
	W: AU, BR, CA, CN, CZ, EE, HU, IL, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	AU 9924787	A1	19990816	AU 1999-24787	19990128 <--
	AU 748818	B2	20020613		
	EP 1049699	A1	20001108	EP 1999-904382	19990128 <--
	EP 1049699	B1	20040421		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
	BR 9908206	A	20001205	BR 1999-8206	19990128 <--
	JP 2002501922	T2	20020122	JP 2000-529335	19990128 <--
	NZ 505079	A	20030829	NZ 1999-505079	19990128 <--
	EP 1344779	A1	20030917	EP 2003-75887	19990128 <--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
	AT 264860	E	20040515	AT 1999-904382	19990128 <--
	TW 520372	B	20030211	TW 1999-88102636	19990223 <--
	US 2003008885	A1	20030109	US 2001-930782	20010816 <--
PRAI	US 1996-23290P	P	19960724	<--	
	US 1997-899242	A2	19970723	<--	
	US 1998-14734	A	19980128	<--	
	US 1998-15001	A	19980128	<--	
	US 1998-15002	A	19980128	<--	
	EP 1999-904382	A3	19990128		

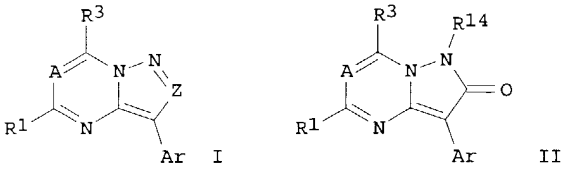
WO 1999-US1824 W 19990128

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 6313124	IC	A61K031-535IC C07D487-04
	NCL	514246000
EP 1344779	ECLA	C07D487/04; C07D487/04 <--
US 2003008885	ECLA	C07D487/04; C07D487/04; C07D487/04 <--

OS MARPAT 135:344507

GI



I II

AB The title compds. [I or II; A = N, CR; Z = N, CR2; Ar = (un)substituted Ph, naphthyl, pyridyl, etc.; R = H, alkyl, alkenyl, etc.; R1 = H, alkyl, alkenyl, etc.; R2 = H, alkyl, alkenyl, etc.; R3 = H, SH, OH, etc.; R14 = C1-10 alkyl, C3-10 alkenyl, C3-10 alkynyl, etc.], corticotropin releasing factor (CRF) antagonists (no data) which are useful in treating anxiety, depression, and other psychiatric, neurol. disorders as well as in treatment of immunol., cardiovascular or heart-related diseases and colonic hypersensitivity associated with psychopathol. disturbance and stress, were prepared and formulated. Thus, treatment of 2,7-dimethyl-8-(2,4-dimethylphenyl)[1,5-a]pyrazolo-1,3,5-triazin-4-one with POCl3 and N,N-dimethylaniline, followed by reaction of the resulting 4-chloro-2,7-dimethyl-8-(2,4-dichlorophenyl)[1,5-a]pyrazolo-1,3,5-triazine with 1,3-dimethoxy-2-aminopropane in EtOH afforded I [A = N; Z = C(Me); R1 = Me; R3 = NHCH(CH2OMe)2; Ar = 2,4-Cl2C6H3].

ST CRF antagonist azolotriazine azolopyrimidine prepn formulation; corticotropin releasing factor antagonist azolotriazine azolopyrimidine prepn

IT Corticotropin releasing factor receptors
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)
(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

IT 202578-49-2P 202579-55-3P 202579-56-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

IT

202578-50-5P	202578-51-6P	202578-52-7P	202578-53-8P	202578-54-9P
202578-55-0P	202578-57-2P	202578-58-3P	202578-59-4P	202578-60-7P
202578-61-8P	202578-62-9P	202578-63-0P	202578-64-1P	202578-65-2P
202578-66-3P	202578-67-4P	202578-68-5P	202578-69-6P	202578-70-9P
202578-71-0P	202578-72-1P	202578-73-2P	202578-74-3P	202578-75-4P
202578-76-5P	202578-77-6P	202578-78-7P	202578-79-8P	202578-80-1P
202578-81-2P	202578-82-3P	202578-83-4P	202578-84-5P	202578-85-6P
202578-86-7P	202578-88-9P	202578-90-3P	202578-92-5P	202578-93-6P
202578-94-7P	202578-95-8P	202578-96-9P	202578-97-0P	202578-98-1P
202578-99-2P	202579-00-8P	202579-01-9P	202579-02-0P	202579-03-1P
202579-04-2P	202579-05-3P	202579-06-4P	202579-08-6P	202579-10-0P
202579-12-2P	202579-14-4P	202579-16-6P	202579-18-8P	202579-20-2P
202579-22-4P	202579-23-5P	202579-25-7P	202579-27-9P	202579-29-1P
202579-30-4P	202579-32-6P	202579-34-8P	202579-36-0P	202579-38-2P
202579-39-3P	202579-41-7P	202579-43-9P	202579-45-1P	202579-46-2P
202579-47-3P	202579-48-4P	202579-49-5P	202579-50-8P	202579-51-9P
202579-52-0P	202579-53-1P	202579-54-2P	202579-57-5P	202579-58-6P
202579-59-7P	202579-60-0P	202579-61-1P	202579-62-2P	202579-63-3P
202579-64-4P	202579-65-5P	202579-66-6P	202579-68-8P	202579-69-9P
202579-70-2P	202579-71-3P	202579-72-4P	202579-73-5P	202579-74-6P
202579-75-7P	202579-76-8P	202579-77-9P	202579-78-0P	202579-79-1P
202579-80-4P	202579-81-5P	202579-82-6P	202579-83-7P	202579-84-8P
202579-85-9P	202579-86-0P	202579-87-1P	202579-88-2P	202579-89-3P
202579-90-6P	202579-91-7P	202579-92-8P	202579-93-9P	202579-94-0P
202579-95-1P	202579-96-2P	202579-97-3P	202579-98-4P	202579-99-5P

202580-00-5P 202580-01-6P 202580-02-7P 202580-03-8P 202580-04-9P
202580-05-0P 202580-06-1P 202580-07-2P 202580-08-3P 202580-09-4P
202580-10-7P 202580-11-8P 202580-12-9P 202580-13-0P 202580-14-1P
202580-15-2P 202580-16-3P 202580-17-4P 202580-18-5P 202580-19-6P
202580-20-9P 202580-21-0P 202580-22-1P 202580-23-2P 202580-24-3P
202580-25-4P 202580-26-5P 202580-27-6P 202580-28-7P 202580-29-8P
261966-75-0P 262297-98-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

IT 105-53-3, Diethyl malonate 141-97-9, Ethyl acetoacetate 616-24-0, 3-Pentylamine 622-79-7, Benzyl azide 1000-84-6 1445-45-0, Trimethyl orthoacetate 34688-71-6, 2,4,6-Trimethylbenzyl cyanide 68429-53-8, 2,4-Dimethylphenylacetonitrile 78531-29-0 202580-72-1 202580-73-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

IT **202580-61-8P**, 1-Cyano-1-(2,4-dimethylphenyl)propan-2-one
202580-62-9P, 5-Amino-4-(2,4-dimethylphenyl)-3-methylpyrazole
202580-64-1P 202580-66-3P 202580-68-5P 202580-70-9P 234778-65-5P
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

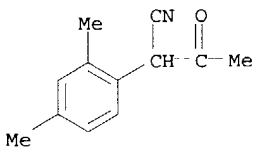
RE.CNT 103 THERE ARE 103 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE

(1) Anon; 1967 HCAPLUS
(2) Anon; JP 4211753 1967
(3) Anon; 1968 HCAPLUS
(4) Anon; 1971 HCAPLUS
(5) Anon; 1971 HCAPLUS
(6) Anon; JP 6157587 1986
(7) Anon; EP 0269859 1988 HCAPLUS
(8) Anon; EP 0300688 1989 HCAPLUS
(9) Anon; EP 0373891 1989 HCAPLUS
(10) Anon; EP 0374448 1990 HCAPLUS
(11) Anon; EP 0395144 1990 HCAPLUS
(12) Anon; EP 0455545 1991 HCAPLUS
(13) Anon; EP 0503099 1992 HCAPLUS
(14) Anon; DE 4243279 1992 HCAPLUS
(15) Anon; WO 9210098 1992 HCAPLUS
(16) Anon; WO 9220642 1992 HCAPLUS
(17) Anon; EP 0521622 1993 HCAPLUS
(18) Anon; EP 0531901 1993 HCAPLUS
(19) Anon; EP 0576350 1993 HCAPLUS
(20) Anon; EP 0591528 1994 HCAPLUS
(21) Anon; EP 0594149 1994 HCAPLUS
(22) Anon; WO 9409017 1994 HCAPLUS
(23) Anon; WO 9413643 1994 HCAPLUS
(24) Anon; WO 9413644 1994 HCAPLUS
(25) Anon; WO 9413661 1994 HCAPLUS
(26) Anon; WO 9413676 1994 HCAPLUS
(27) Anon; WO 9413677 1994 HCAPLUS
(28) Anon; EP 0662477 1995 HCAPLUS
(29) Anon; EP 0714898 1995 HCAPLUS
(30) Anon; WO 9500507 1995 HCAPLUS
(31) Anon; WO 9511880 1995 HCAPLUS
(32) Anon; WO 9532710 1995 HCAPLUS
(33) Anon; WO 9533727 1995 HCAPLUS
(34) Anon; WO 9533750 1995 HCAPLUS
(35) Anon; WO 9534563 1995 HCAPLUS
(36) Anon; EP 0729758 1996 HCAPLUS
(37) Anon; WO 9535298 1996 HCAPLUS
(38) Anon; WO 9619452 1996 HCAPLUS
(39) Anon; WO 9623783 1996 HCAPLUS
(40) Anon; WO 9635689 1996 HCAPLUS
(41) Anon; WO 9639388 1996 HCAPLUS
(42) Anon; WO 9639400 1996 HCAPLUS
(43) Anon; EP 0773023 1997 HCAPLUS
(44) Anon; EP 0778277 1997 HCAPLUS
(45) Anon; EP 0812831 1997 HCAPLUS
(46) Anon; WO 9700868 1997 HCAPLUS
(47) Anon; WO 9714684 1997 HCAPLUS
(48) Anon; WO 9729109 1997 HCAPLUS

(49) Anon; WO 9729110 1997 HCAPLUS
(50) Anon; WO 9808821 1998 HCAPLUS
(51) Anon; WO 9808846 1998 HCAPLUS
(52) Anon; WO 9808847 1998 HCAPLUS
(53) Anon; Arch Pharm (Weinheim) 1987, V320, P487
(54) Arato; Biol Psychiatry 1989, V25, P355 MEDLINE
(55) Banki; Am J Psychiatry 1987, V144, P873 MEDLINE
(56) Bantick; US 5428044 1995 HCAPLUS
(57) Barker; US 5089499 1992 HCAPLUS
(58) Battaglia; Synapse 1987, V1, P572 HCAPLUS
(59) Berridge; Hormones and Behavior 1987, V21, P393 HCAPLUS
(60) Berridge; Regulatory Peptides 1986, V16, P83 HCAPLUS
(61) Blalock; Physiological Reviews 1989, V69(1), P1 HCAPLUS
(62) Britton; Life Sciences 1982, V31, P363 HCAPLUS
(63) Britton; Psychopharmacology 1985, V86, P170 HCAPLUS
(64) Britton; Psychopharmacology 1988, V94, P306 HCAPLUS
(65) Bussler; US 5484760 1996 HCAPLUS
(66) Courtemanche; US 5464847 1995 HCAPLUS
(67) de Souza; Corticotropin-Releasing Factor:Basic and Clinical Studies of a Neuropeptide P221
(68) de Souza; Hospital Practice 1988, P59 MEDLINE
(69) de Souza; Journal of Neuroscience 1985, V5(12), P3189 HCAPLUS
(70) Dunn; Brain Research Reviews 1990, V15, P71 HCAPLUS
(71) Eicken; US 4567263 1986 HCAPLUS
(72) France; Biol Psychiatry 1988, V23, P86 MEDLINE
(73) Gennaro; Remington's Pharmaceutical Sciences, 17th ed P1418
(74) Gold; New Eng J Med 1986, V314(21), P1329 MEDLINE
(75) Grigoriadis; Neuropsychopharmacology 1989, V2(1), P53 HCAPLUS
(76) Hashimoto; US 5137887 1992 HCAPLUS
(77) Himmelsbach; US 5463071 1995 HCAPLUS
(78) Himmler; US 4990647 1991 HCAPLUS
(79) Koob; Perspectives on Behavioral Medicine 1985, V2, P39
(80) Kruger; US 4892576 1990 HCAPLUS
(81) Maquestiau; Bull Soc Chim Belg 1992, V101(2) HCAPLUS
(82) Morley; Life Sciences 1987, V41, P527 HCAPLUS
(83) Nemeroff; Arch Gen Psychiatry 1988, V45, P577 MEDLINE
(84) Nemeroff; Science 1984, V226, P1342 MEDLINE
(85) Nugent; US 5397774 1995 HCAPLUS
(86) O'Brien; US 3910907 1975 HCAPLUS
(87) O'Brien; 1976 HCAPLUS
(88) Rivier; Proc Natl Acad Sci 1983, V80, P4851 HCAPLUS
(89) Rooney; US 3995039 1976 HCAPLUS
(90) Sapolsky; Arch Gen Psychiatry 1989, V46, P1047 MEDLINE
(91) Schonafinger; US 5486531 1996 HCAPLUS
(92) Senga; 1982 HCAPLUS
(93) Senga; J Med Chem 1982, V25, P243 HCAPLUS
(94) Senga; J Med Chem 1982, V25, P243 HCAPLUS
(95) Springer; US 3920652 1975 HCAPLUS
(96) Springer; US 4021556 1977 HCAPLUS
(97) Swerdlow; Psychopharmacology 1986, V88, P147 HCAPLUS
(98) Trost; Comprehensive Organic Synthesis V3, P481
(99) Trost; Comprehensive Organic Synthesis V7, P762
(100) Vale; Recent Progress in Hormone Research 1983, V39, P245 HCAPLUS
(101) Vale; Science 1981, V213, P1394 HCAPLUS
(102) Vinogradoff; US 4997940 1991 HCAPLUS
(103) Yuan; US 5723608 1998 HCAPLUS

IT **202580-61-8P**, 1-Cyano-1-(2,4-dimethylphenyl)propan-2-one
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of azolotriazines and -pyrimidines as corticotropin releasing factor (CRF) antagonists)

RN 202580-61-8 HCAPLUS
CN Benzeneacetonitrile, .alpha.-acetyl-2,4-dimethyl- (9CI) (CA INDEX NAME)



L28 ANSWER 6 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:131201 HCAPLUS

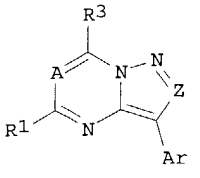
DN 134:178572
ED Entered STN: 22 Feb 2001
TI Preparation of azolo triazines and pyrimidines as corticotropin releasing factor (CRF) antagonists
IN He, Liqi; Gilligan, Paul; Chorvat, Robert; Arvanitis, Argyrios Georgios
PA Dupont Pharmaceuticals Co., USA
SO U.S., 90 pp., Cont.-in-part of U. S. Ser. No. 899,242.
CODEN: USXXAM
DT **Patent**
LA English
IC ICM C07D487-04
ICS C07D251-72; A61K031-53
NCL 514246000
CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 2, 63
FAN.CNT 5

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	US 6191131	B1	20010220	US 1998-15002	19980128	<--
	US 6124289	A	20000926	US 1997-899242	19970723	<--
	ZA 9706603	A	19990125	ZA 1997-6603	19970724	<--
	US 6136809	A	20001024	US 1998-14999	19980128	<--
	LT 4680	B	20000725	LT 1999-8	19990125	<--
	CA 2314613	AA	19990805	CA 1999-2314613	19990128	<--
	WO 9938868	A1	19990805	WO 1999-US1824	19990128	<--
	W: AU, BR, CA, CN, CZ, EE, HU, IL, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE					
	AU 9924787	A1	19990816	AU 1999-24787	19990128	<--
	AU 748818	B2	20020613			
	EP 1049699	A1	20001108	EP 1999-904382	19990128	<--
	EP 1049699	B1	20040421			
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO					
	BR 9908206	A	20001205	BR 1999-8206	19990128	<--
	JP 2002501922	T2	20020122	JP 2000-529335	19990128	<--
	NZ 505079	A	20030829	NZ 1999-505079	19990128	<--
	EP 1344779	A1	20030917	EP 2003-75887	19990128	<
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO					
	AT 264860	E	20040515	AT 1999-904382	19990128	<--
	TW 520372	B	20030211	TW 1999-88102636	19990223	<--
	US 6358950	B1	20020319	US 2000-696759	20001026	<--
PRAI	US 1996-23290P	P	19960724	<--		
	US 1997-899242	A2	19970723	<--		
	US 1998-14734	A	19980128	<--		
	US 1998-15001	A	19980128	<--		
	US 1998-15002	A	19980128	<--		
	EP 1999-904382	A3	19990128			
	WO 1999-US1824	W	19990128			

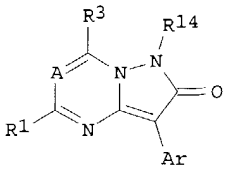
CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES	
US 6191131	ICM	C07D487-04	
	ICS	C07D251-72; A61K031-53	
	NCL	514246000	
EP 1344779	ECLA	C07D487/04; C07D487/04	<--

OS MARPAT 134:178572
GI



I



II

AB The title compds. [I or II; A = N, CR; Z = N, CR2; Ar = (un)substituted Ph, naphthyl, pyridyl, etc.; R = H, alk(en/yn)yl, halo, etc.; R1, R2 = H, alk(en/yn)yl, halo, etc.; R3 = H, SH, aryl, etc.; R14 = (un)substituted alk(en/yn)yl, cycloalkyl(alkyl)], useful in treating CRF-related

disorders, particularly anxiety, depression, and other psychiatric, neurol. disorders as well as treatment of immunol., cardiovascular or heart-related diseases and colonic hypersensitivity associated with psychopathol. disturbance and stress, were prepared and formulated. For instance, 5-amino-4-(2-chloro-4-methylphenyl)-3-methylpyrazole was cyclized with Et acetoacetate in AcOH to give 42% 7-hydroxy-2,5-dimethyl-3-(2-chloro-4-methylphenyl)pyrazolo[1,5-a]pyrimidine. The latter was treated with POCl3 and PhNEt2 to give the 7-chloro analog (84%), which reacted with 3-pentylamine to give 60% title compound I [A = CH; R1 = Me; R3 = NHCHEt2; Z = CMe; Ar = 2-Cl-4-MeC6H3]. The compds. I are effective at 0.002-200 mg/kg/day.

ST azolo triazine pyrimidine prepn formulation CRF antagonist; corticotropin releasing factor antagonist pyrazolopyrimidine pyrazolotriazine prepn antidepressant anxiolytic; azolotriazine prepn formulation CRF receptor antagonist; azolopyrimidine prepn formulation CRF receptor antagonist

IT Antidepressants
Anxiolytics
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT Corticotropin releasing factor receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT 202578-49-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT
202578-50-5P	202578-51-6P	202578-52-7P	202578-53-8P	202578-54-9P
202578-55-0P	202578-58-3P	202578-59-4P	202578-60-7P	202578-61-8P
202578-62-9P	202578-63-0P	202578-64-1P	202578-65-2P	202578-66-3P
202578-67-4P	202578-68-5P	202578-69-6P	202578-70-9P	202578-71-0P
202578-72-1P	202578-73-2P	202578-74-3P	202578-75-4P	202578-76-5P
202578-77-6P	202578-78-7P	202578-79-8P	202578-80-1P	202578-81-2P
202578-82-3P	202578-83-4P	202578-84-5P	202578-85-6P	202578-86-7P
202578-88-9P	202578-90-3P	202578-92-5P	202578-93-6P	202578-94-7P
202578-95-8P	202578-96-9P	202578-97-0P	202578-98-1P	202578-99-2P
202579-00-8P	202579-01-9P	202579-02-0P	202579-03-1P	202579-04-2P
202579-05-3P	202579-06-4P	202579-08-6P	202579-10-0P	202579-12-2P
202579-14-4P	202579-16-6P	202579-18-8P	202579-20-2P	202579-22-4P
202579-23-5P	202579-25-7P	202579-27-9P	202579-29-1P	202579-30-4P
202579-32-6P	202579-34-8P	202579-36-0P	202579-38-2P	202579-39-3P
202579-41-7P	202579-43-9P	202579-45-1P	202579-46-2P	202579-47-3P
202579-48-4P	202579-49-5P	202579-50-8P	202579-51-9P	202579-52-0P
202579-53-1P	202579-54-2P	202579-55-3P	202579-56-4P	202579-57-5P
202579-58-6P	202579-59-7P	202579-60-0P	202579-61-1P	202579-62-2P
202579-63-3P	202579-64-4P	202579-65-5P	202579-66-6P	202579-68-8P
202579-69-9P	202579-70-2P	202579-71-3P	202579-72-4P	202579-73-5P
202579-74-6P	202579-75-7P	202579-76-8P	202579-77-9P	202579-78-0P
202579-79-1P	202579-80-4P	202579-81-5P	202579-82-6P	202579-83-7P
202579-84-8P	202579-85-9P	202579-86-0P	202579-87-1P	202579-88-2P
202579-89-3P	202579-90-6P	202579-91-7P	202579-92-8P	202579-93-9P
202579-94-0P	202579-95-1P	202579-96-2P	202579-97-3P	202579-98-4P
202579-99-5P	202580-00-5P	202580-01-6P	202580-02-7P	202580-04-9P
202580-05-0P	202580-06-1P	202580-07-2P	202580-08-3P	202580-09-4P
202580-10-7P	202580-11-8P	202580-12-9P	202580-13-0P	202580-14-1P
202580-15-2P	202580-16-3P	202580-17-4P	202580-18-5P	202580-19-6P
202580-20-9P	202580-21-0P	202580-22-1P	202580-23-2P	202580-24-3P
202580-25-4P	202580-26-5P	202580-27-6P	202580-28-7P	202580-29-8P
202580-30-1P	202580-32-3P	202580-35-6P	202580-36-7P	202580-37-8P
202580-38-9P	202580-39-0P	202580-40-3P	202580-41-4P	234772-66-8P
234772-67-9P	234772-68-0P	234772-69-1P	234772-70-4P	234772-71-5P
234772-72-6P	234772-73-7P	234772-74-8P	234772-75-9P	234772-76-0P
234772-77-1P	234772-78-2P	234772-79-3P	234772-80-6P	234772-81-7P
234772-82-8P	234772-83-9P	234772-84-0P	234772-86-2P	234772-87-3P
234772-88-4P	234772-89-5P	234772-90-8P	234772-91-9P	234772-92-0P
234772-93-1P	234772-94-2P	234772-95-3P	234772-96-4P	234772-97-5P
234772-98-6P	234772-99-7P	234773-00-3P	234773-01-4P	234773-02-5P
234773-03-6P	234773-04-7P	234773-05-8P	234773-07-0P	234773-09-2P
234773-11-6P	234773-13-8P	234773-15-0P	234773-16-1P	234773-18-3P
234773-19-4P	234773-20-7P	234773-21-8P	234773-22-9P	234773-23-0P
234773-24-1P	234773-25-2P	234773-26-3P	234773-27-4P	234773-29-6P
234773-31-0P	234773-33-2P	234773-35-4P	234773-37-6P	234773-38-7P
234773-40-1P	234773-42-3P	234773-44-5P	234773-46-7P	234773-48-9P
234773-50-3P	234773-51-4P	234773-52-5P	234773-53-6P	

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT 234773-54-7P 234773-56-9P 234773-58-1P 234773-60-5P 234773-62-7P
234773-64-9P 234773-66-1P 234773-68-3P 234773-70-7P 234773-72-9P
234773-74-1P 234773-75-2P 234773-76-3P 234773-77-4P 234773-78-5P
234773-79-6P 234773-80-9P 234773-81-0P 234773-82-1P 234773-83-2P
234773-84-3P 234773-85-4P 234773-86-5P 234773-87-6P 234773-88-7P
234773-89-8P 234773-90-1P 234773-91-2P 234773-92-3P 234773-93-4P
234773-94-5P 234773-95-6P 234773-96-7P 234773-97-8P 234773-98-9P
234773-99-0P 234774-00-6P 234774-01-7P 234774-02-8P 234774-03-9P
234774-04-0P 234774-05-1P 234774-06-2P 234774-07-3P 234774-08-4P
234774-09-5P 234774-10-8P 234774-11-9P 234774-12-0P 234774-13-1P
234774-14-2P 234774-15-3P 234774-16-4P 234774-17-5P 234774-18-6P
234774-19-7P 234774-20-0P 234774-21-1P 234774-22-2P 234774-23-3P
234774-24-4P 234774-25-5P 234774-26-6P 234774-27-7P 234774-28-8P
234774-29-9P 234774-30-2P 234774-31-3P 234774-32-4P 234774-33-5P
234774-34-6P 234774-35-7P 234774-36-8P 234774-37-9P 234774-38-0P
234774-39-1P 234774-40-4P 234774-41-5P 234774-42-6P 234774-43-7P
234774-44-8P 234774-45-9P 234774-46-0P 234774-47-1P 234774-48-2P
234774-49-3P 234774-50-6P 234774-51-7P 234774-52-8P 234774-53-9P
234774-54-0P 234774-55-1P 234774-57-3P 234774-59-5P 234774-61-9P
234774-63-1P 234774-64-2P 234774-65-3P 234774-66-4P 234774-67-5P
234774-69-7P 234774-74-4P 234774-76-6P 234774-78-8P 234774-80-2P
234774-82-4P 234774-84-6P 234774-86-8P 234774-88-0P 234774-89-1P
234774-91-5P 234774-92-6P 234774-93-7P 234774-94-8P 234774-95-9P
234774-96-0P 234774-97-1P 234774-98-2P 234774-99-3P 234775-00-9P
234775-01-0P 234775-02-1P 234775-03-2P 234775-04-3P 234775-05-4P
234775-06-5P 234775-07-6P 234775-08-7P 234775-09-8P 234775-10-1P
234775-11-2P 234775-12-3P 234775-13-4P 234775-14-5P 234775-16-7P
234775-17-8P 234775-18-9P 234775-19-0P 234775-20-3P 234775-21-4P
234775-22-5P 234775-23-6P 234775-24-7P 234775-25-8P 234775-26-9P
234775-27-0P 234775-28-1P 234775-29-2P 234775-30-5P 234775-31-6P
234775-32-7P 234775-33-8P 234775-34-9P 234775-35-0P 234775-36-1P
234775-37-2P 234775-38-3P 234775-39-4P 234775-40-7P 234775-41-8P
234775-42-9P 234775-43-0P 234775-44-1P 234775-45-2P 234775-46-3P
234775-47-4P 234775-48-5P 234775-49-6P 234775-50-9P 234775-51-0P
234775-52-1P 234775-53-2P 234775-54-3P 234775-55-4P 234775-56-5P
234775-57-6P 234775-58-7P 234775-59-8P 234775-60-1P 234775-61-2P
234775-62-3P 234775-63-4P 234775-64-5P 234775-65-6P 234775-66-7P
234775-67-8P 234775-68-9P 234775-69-0P 234775-70-3P 234775-71-4P
234775-72-5P 234775-73-6P 234775-74-7P 234775-76-9P 234775-77-0P
234775-78-1P 234775-79-2P 234775-80-5P 234775-81-6P 234775-82-7P
234775-83-8P 234775-84-9P 234775-85-0P 234775-86-1P 234775-87-2P
234775-88-3P 234775-89-4P 234775-90-7P 234775-91-8P 234775-92-9P
234775-93-0P 234775-94-1P 234775-95-2P 234775-96-3P 234775-97-4P
234775-98-5P 234775-99-6P 234776-00-2P 234776-01-3P 234776-02-4P
234776-03-5P 234776-04-6P 234776-05-7P 234776-06-8P 234776-07-9P
234776-08-0P 234776-09-1P 234776-10-4P 234776-11-5P 234776-12-6P
234776-13-7P 234776-14-8P 234776-15-9P 234776-16-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT 234776-17-1P 234776-18-2P 234776-19-3P 234776-20-6P 234776-21-7P
234776-22-8P 234776-23-9P 234776-24-0P 234776-26-2P 234776-27-3P
234776-28-4P 234776-29-5P 234776-30-8P 234776-31-9P 234776-32-0P
234776-33-1P 234776-34-2P 234776-35-3P 234776-36-4P 234776-37-5P
234776-38-6P 234776-39-7P 234776-40-0P 234776-41-1P 234776-42-2P
234776-43-3P 234776-44-4P 234776-45-5P 234776-46-6P 234776-47-7P
234776-48-8P 234776-49-9P 234776-50-2P 234776-51-3P 234776-52-4P
234776-53-5P 234776-54-6P 234776-55-7P 234776-56-8P 234776-57-9P
234776-58-0P 234776-59-1P 234776-60-4P 234776-61-5P 234776-62-6P
234776-63-7P 234776-64-8P 234776-65-9P 234776-66-0P 234776-67-1P
234776-68-2P 234776-69-3P 234778-55-3P 234778-56-4P 234778-57-5P
234778-58-6P 234778-59-7P 234778-60-0P 234778-61-1P 261966-75-0P
326821-49-2P 326821-82-3P 326821-83-4P 326821-84-5P 326821-85-6P
326821-86-7P 326821-87-8P 326821-88-9P 326821-89-0P 326821-90-3P
326821-91-4P 326821-93-6P 326821-94-7P 326821-95-8P 326821-96-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

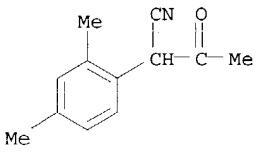
IT 105-53-3, Diethyl malonate 105-58-8, Diethyl carbonate 141-97-9, Ethyl acetoacetate 616-24-0, 3-Pentylamine 622-79-7, Benzyl azide
1445-45-0, Trimethyl orthoacetate 2208-07-3 34688-71-6,

2,4,6-Trimethylbenzyl cyanide 68429-53-8, 2,4-Dimethylphenylacetonitrile
78531-29-0 202580-72-1 202580-73-2 326821-97-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)
IT 1000-84-6P **202580-61-8P** 202580-62-9P 202580-64-1P
202580-66-3P 202580-68-5P 202580-70-9P 234778-65-5P
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)
RE.CNT 93 THERE ARE 93 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Anon; 1967, 28, HCAPLUS
(2) Anon; JP 4211753 1967
(3) Anon; 1968, 28, HCAPLUS
(4) Anon; 1971, 28, HCAPLUS
(5) Anon; 1971, 28, HCAPLUS
(6) Anon; JP 6157587 1986
(7) Anon; EP 0269859 1988 HCAPLUS
(8) Anon; EP 0300688 1989 HCAPLUS
(9) Anon; EP 0373891 1989 HCAPLUS
(10) Anon; EP 0374448 1990 HCAPLUS
(11) Anon; EP 0395144 1990 HCAPLUS
(12) Anon; EP 0455545 1991 HCAPLUS
(13) Anon; EP 0503099 1992 HCAPLUS
(14) Anon; WO 9220642 1992 HCAPLUS
(15) Anon; EP 0521622 1993 HCAPLUS
(16) Anon; EP 0531901 1993 HCAPLUS
(17) Anon; EP 0576350 1993 HCAPLUS
(18) Anon; EP 0591528 1994 HCAPLUS
(19) Anon; EP 0594149 1994 HCAPLUS
(20) Anon; WO 9409017 1994 HCAPLUS
(21) Anon; WO 9413643 1994 HCAPLUS
(22) Anon; WO 9413644 1994 HCAPLUS
(23) Anon; WO 9413661 1994 HCAPLUS
(24) Anon; WO 9413676 1994 HCAPLUS
(25) Anon; WO 9413677 1994 HCAPLUS
(26) Anon; EP 0662477 1995 HCAPLUS
(27) Anon; EP 0714898 1995 HCAPLUS
(28) Anon; WO 9500507 1995 HCAPLUS
(29) Anon; WO 9511880 1995 HCAPLUS
(30) Anon; WO 9533727 1995 HCAPLUS
(31) Anon; WO 9533750 1995 HCAPLUS
(32) Anon; WO 9534563 1995 HCAPLUS
(33) Anon; EP 0729758 1996 HCAPLUS
(34) Anon; WO 9535298 1996 HCAPLUS
(35) Anon; WO 9619452 1996 HCAPLUS
(36) Anon; WO 9623783 1996 HCAPLUS
(37) Anon; WO 9635689 1996 HCAPLUS
(38) Anon; WO 9639388 1996 HCAPLUS
(39) Anon; WO 9639400 1996 HCAPLUS
(40) Anon; EP 0773023 1997 HCAPLUS
(41) Anon; EP 0778277 1997 HCAPLUS
(42) Anon; EP 0812831 1997 HCAPLUS
(43) Anon; Remington's Pharmaceutical Sciences 17th P1418
(44) Arato; Biol Psychiatry 1989, V25, P355 MEDLINE
(45) Baker; US 5089499 1992 HCAPLUS
(46) Banki; Am J Psychiatry 1987, V144, P873 MEDLINE
(47) Bantick; US 5428044 1995 HCAPLUS
(48) Battaglia; Synapse 1987, V1, P572 HCAPLUS
(49) Berridge; Hormones and Behavior 1987, V21, P393 HCAPLUS
(50) Berridge; Regulatory Peptides 1986, V16, P83 HCAPLUS
(51) Blalock; Physiological Reviews 1989, V69(1), P1 HCAPLUS
(52) Britton; Life Sciences 1982, V31, P363 HCAPLUS
(53) Britton; Psychopharmacology 1985, V86, P170 HCAPLUS
(54) Britton; Psychopharmacology 1988, V94, P306 HCAPLUS
(55) Bussler; US 5484760 1996 HCAPLUS
(56) De Souza; Corticotropin Releasing Factor: Basic and Clinical Studies of a Neuropeptide 1990, P221
(57) De Souza; Hospital Practice 1988, P59 MEDLINE
(58) De Souza; Journal of Neuroscience 1985, V5(12), P3189 HCAPLUS
(59) Dunn; Brain Research Reviews 1990, V15, P71 HCAPLUS
(60) Eicken; US 4567263 1986 HCAPLUS
(61) France; Biol Psychiatry 1988, V23, P86 MEDLINE
(62) Gold; New Eng J Med 1986, V314(21), P1329 MEDLINE
(63) Grigoriadis; Neuropsychopharmacology 1989, V2(1), P53 HCAPLUS
(64) Hashimoto; US 5137887 1992 HCAPLUS

(65) Himmelsbach; US 5463071 1995 HCAPLUS
(66) Himmler; US 4990647 1991 HCAPLUS
(67) Joshi; Journal f prakt Chemie 1979, P341 HCAPLUS
(68) Koob; Perspectives on Behavioral Medicine 1985, V2, P39
(69) Kruger; US 4892576 1990 HCAPLUS
(70) Maquestiau; Bull Soc Chim Belg 1992, V101(2) HCAPLUS
(71) Morley; Life Sciences 1987, V41, P527 HCAPLUS
(72) Nemeroff; Arch Gen Psychiatry 1988, V45, P577 MEDLINE
(73) Nemeroff; Science 1984, V226, P1342 MEDLINE
(74) Nugent; US 5397774 1995 HCAPLUS
(75) O'Brien; US 3910907 1975 HCAPLUS
(76) O'Brien; J Heterocyclic Chem 1985, V22, P601
(77) Rivier; Proc Natl Acad Sci 1983, V80, P4851 HCAPLUS
(78) Rooney; US 3995039 1976 HCAPLUS
(79) Sapolsky; Arch Gen Psychiatry 1989, V46, P1047 MEDLINE
(80) Schonafinger; US 5486531 1996 HCAPLUS
(81) Senga; J Med Chem 1981, V24, P610 HCAPLUS
(82) Senga; J Med Chem 1982, V25, P243 HCAPLUS
(83) Springer; US 3920652 1975 HCAPLUS
(84) Springer; US 4021556 1977 HCAPLUS
(85) Springer; Journal of Medicinal Chemistry 1976, V19(2), P291 HCAPLUS
(86) Swerdlow; Psychopharmacology 1986, V88, P147 HCAPLUS
(87) Trost; Comprehensive Organic Synthesis 1991, V3, P481
(88) Trost; Comprehensive Organic Synthesis 1991, V7, P762
(89) Vale; Recent Progress in Hormone Research 1983, V39, P245 HCAPLUS
(90) Vale; Science 1981, P213
(91) Vinogradoff; US 4997940 1991 HCAPLUS
(92) Weinheim; Arch Pharm 1987, V320, P487
(93) Yuan; US 5723608 1998 HCAPLUS

IT **202580-61-8P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

RN 202580-61-8 HCAPLUS
CN Benzeneacetonitrile, .alpha.-acetyl-2,4-dimethyl- (9CI) (CA INDEX NAME)



L28 ANSWER 7 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:307132 HCAPLUS
DN 132:321873
ED Entered STN: 12 May 2000
TI Azolo triazines and pyrimidines useful as corticotropin releasing factor (CRF) antagonists
IN Gilligan, Paul; Chorvat, Robert; Arvanitis, Argyrios Georgios
PA DuPont Pharmaceuticals Co., USA
SO U.S., 86 pp., Cont.-in-part of U.S. Ser. No. 899,242.
CODEN: USXXAM
DT **Patent**
LA English
IC ICM A61K031-505
ICS C07D487-04
NCL 514258000
CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 2

FAN.CNT 5

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 6060478	A	20000509	US 1998-15001	19980128 <--
US 6124289	A	20000926	US 1997-899242	19970723 <--
ZA 9706603	A	19990125	ZA 1997-6603	19970724 <--
US 6136809	A	20001024	US 1998-14999	19980128 <--
LT 4680	B	20000725	LT 1999-8	19990125 <--
CA 2314613	AA	19990805	CA 1999-2314613	19990128 <--
WO 9938868	A1	19990805	WO 1999-US1824	19990128 <--

W: AU, BR, CA, CN, CZ, EE, HU, IL, JP, KR, LT, LV, MX, NO, NZ, PL, RO, SG, SI, SK, UA, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,

PT, SE

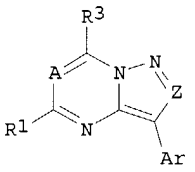
AU 9924787	A1	19990816	AU 1999-24787	19990128	<--
AU 748818	B2	20020613			
EP 1049699	A1	20001108	EP 1999-904382	19990128	<--
EP 1049699	B1	20040421			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO					
BR 9908206	A	20001205	BR 1999-8206	19990128	<--
JP 2002501922	T2	20020122	JP 2000-529335	19990128	<--
NZ 505079	A	20030829	NZ 1999-505079	19990128	<--
EP 1344779	A1	20030917	EP 2003-75887	19990128	<--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO					
AT 264860	E	20040515	AT 1999-904382	19990128	<--
TW 520372	B	20030211	TW 1999-88102636	19990223	<--
PRAI US 1996-23290P	P	19960724	<--		
US 1997-899242	A2	19970723	<--		
US 1998-14734	A	19980128	<--		
US 1998-15001	A	19980128	<--		
US 1998-15002	A	19980128	<--		
EP 1999-904382	A3	19990128			
WO 1999-US1824	W	19990128			

CLASS

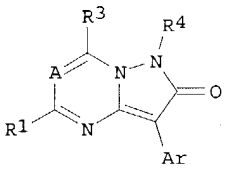
PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES	
US 6060478	ICM	A61K031-505	
	ICS	C07D487-04	
	NCL	514258000	
US 6060478	ECLA	C07D487/04; C07D487/04; C07D487/04	<--
EP 1344779	ECLA	C07D487/04; C07D487/04	<--

OS MARPAT 132:321873

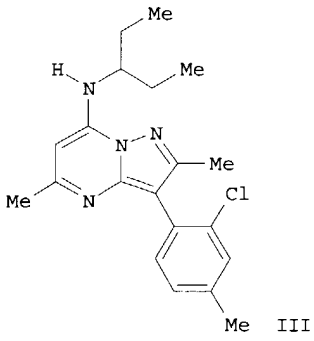
GI



I



II



III

AB Corticotropin releasing factor (CRF) antagonists (no data) of formulas I and II are disclosed [wherein A = N or CR; Z = N or CR2; Ar = (un)substituted Ph, naphthyl, pyridyl, pyrimidinyl, indanyl, tetralinyl, addnl. selected heterocycles; R = H, alk(en/yn)yl, cycloalkyl(alkyl), halo, cyano, haloalkyl; R1, R2 = H, groups listed for R, NH2 or derivs., OH or derivs., SH or derivs., addnl. substituted alkyls; R3 = H, OH or derivs., SH or derivs., acyl, CO2H or esters, NH2 or derivs., aryl, heteroaryl, alk(en/yn)yl, etc.; R4 = (un)substituted alk(en/yn)yl or cycloalkyl(alkyl)]. The compds. are of use in the treatment of CRF-related disorders, particularly anxiety and depression, as well as other psychiatric, neurol., immunol., cardiovascular, and psychopathol. disorders. For instance, 5-amino-4-(2-chloro-4-methylphenyl)-3-

methylpyrazole was cyclized with Et acetoacetate in AcOH to give 42% 7-hydroxy-5-methyl-3-(2-chloro-4-methylphenyl)pyrazolo[1,5-a]pyrimidine. The latter was treated with POCl3 and PhNEt2 to give the 7-chloro analog (84%), which reacted with 3-pentylamine to give 60% title compound III.

ST azolo triazine pyrimidine prepn CRF antagonist; corticotropin releasing factor antagonist pyrazolopyrimidine pyrazolotriazine prepn antidepressant anxiolytic; azolotriazine azolopyrimidine prepn CRF receptor antagonist

IT Drugs
(gastrointestinal; preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT Intestine, disease
(irritable bowel syndrome, treatment; preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT Anti-inflammatory agents
Antidepressants
Anxiolytics
Cardiovascular agents
Immunomodulators
Nervous system agents
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT Corticotropin releasing factor receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT 1000-84-6P 202578-49-2P 202578-50-5P 202579-55-3P 202579-56-4P
202580-61-8P, 1-Cyano-1-(2,4-dimethylphenyl)propan-2-one
202580-62-9P 202580-64-1P 202580-66-3P 202580-68-5P 202580-69-6P
202580-70-9P 234778-65-5P
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(intermediate; preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT 9015-71-8, Corticotropin releasing factor
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT 105-53-3, Diethyl malonate 105-58-8 141-78-6, Acetic acid ethyl ester, reactions 141-97-9 616-24-0, 3-Pentylamine 622-79-7, Benzyl azide 1445-45-0, Trimethyl orthoacetate 2208-07-3 34688-71-6, 2,4,6-Trimethylbenzyl cyanide 68429-53-8, 2,4-Dimethylphenylacetonitrile 78531-29-0, 1,3-Dimethoxy-2-aminopropane 202580-72-1 202580-73-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT 202578-52-7P 202578-53-8P 202578-54-9P 202578-55-0P 202578-57-2P
202578-58-3P 202578-59-4P 202578-60-7P 202578-61-8P 202578-62-9P
202578-63-0P 202578-64-1P 202578-65-2P 202578-66-3P 202578-67-4P
202578-68-5P 202578-69-6P 202578-70-9P 202578-71-0P 202578-72-1P
202578-73-2P 202578-74-3P 202578-75-4P 202578-76-5P 202578-77-6P
202578-78-7P 202578-79-8P 202578-80-1P 202578-81-2P 202578-82-3P
202578-83-4P 202578-84-5P 202578-85-6P 202578-86-7P 202578-88-9P
202578-90-3P 202578-92-5P 202578-93-6P 202578-94-7P 202578-95-8P
202578-96-9P 202578-97-0P 202578-98-1P 202578-99-2P 202579-00-8P
202579-01-9P 202579-02-0P 202579-03-1P 202579-04-2P 202579-05-3P
202579-06-4P 202579-08-6P 202579-10-0P 202579-12-2P 202579-14-4P
202579-16-6P 202579-18-8P 202579-20-2P 202579-22-4P 202579-23-5P
202579-25-7P 202579-27-9P 202579-29-1P 202579-30-4P 202579-32-6P
202579-34-8P 202579-36-0P 202579-38-2P 202579-39-3P 202579-41-7P
202579-43-9P 202579-45-1P 202579-46-2P 202579-47-3P 202579-48-4P
202579-49-5P 202579-50-8P 202579-51-9P 202579-52-0P 202579-53-1P
202579-54-2P 202579-57-5P 202579-58-6P 202579-59-7P 202579-60-0P
202579-61-1P 202579-62-2P 202579-63-3P 202579-64-4P 202579-65-5P
202579-66-6P 202579-68-8P 202579-69-9P 202579-70-2P 202579-71-3P
202579-72-4P 202579-73-5P 202579-74-6P 202579-75-7P 202579-76-8P
202579-77-9P 202579-78-0P 202579-79-1P 202579-80-4P 202579-81-5P
202579-82-6P 202579-83-7P 202579-84-8P 202579-85-9P 202579-86-0P
202579-87-1P 202579-88-2P 202579-89-3P 202579-90-6P 202579-91-7P
202579-92-8P 202579-93-9P 202579-94-0P 202579-95-1P 202579-96-2P
202579-97-3P 202579-98-4P 202579-99-5P 202580-00-5P 202580-01-6P
202580-02-7P 202580-03-8P 202580-04-9P 202580-05-0P 202580-06-1P
202580-07-2P 202580-08-3P 202580-09-4P 202580-10-7P 202580-11-8P
202580-12-9P 202580-13-0P 202580-14-1P 202580-15-2P 202580-16-3P
202580-17-4P 202580-18-5P 202580-19-6P 202580-20-9P 202580-21-0P
202580-22-1P 202580-23-2P 202580-24-3P 202580-25-4P 202580-26-5P
202580-27-6P 202580-28-7P 202580-29-8P 202580-31-2P 202580-32-3P
202580-34-5P 202580-35-6P 202580-36-7P 202580-37-8P 202580-39-0P

202580-53-8P 202580-54-9P 202580-56-1P 202580-57-2P 202580-58-3P
202580-59-4P 202580-60-7P 234776-70-6P 234776-71-7P 234776-72-8P
234776-73-9P 234776-74-0P 234776-75-1P 234776-76-2P 234776-77-3P
234776-78-4P 234776-79-5P 234776-80-8P 234776-81-9P 234776-82-0P
234776-83-1P 234776-84-2P 234776-85-3P 234776-86-4P 234776-87-5P
234776-88-6P 234776-89-7P 234776-90-0P 234776-91-1P 234776-92-2P
234776-93-3P 234776-94-4P 234776-95-5P 234776-96-6P 234776-97-7P
234776-98-8P 234776-99-9P 234777-00-5P 234777-01-6P 234777-02-7P
234777-03-8P 234777-04-9P 234777-05-0P 234777-06-1P 234777-07-2P
234777-08-3P 234777-09-4P 234777-10-7P 234777-11-8P 234777-12-9P
234777-13-0P 234777-14-1P 234777-15-2P 234777-16-3P 234777-17-4P
234777-18-5P 234777-19-6P 234777-20-9P 234777-21-0P 234777-22-1P
234777-23-2P 234777-24-3P 234777-25-4P 234777-26-5P 234777-27-6P
234777-28-7P 234777-29-8P 234777-30-1P 234777-31-2P 234777-32-3P
234777-33-4P 234777-34-5P 234777-35-6P 234777-36-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compound; preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

IT 234777-37-8P 234777-38-9P 234777-39-0P 234777-40-3P 234777-42-5P
234777-43-6P 234777-44-7P 234777-45-8P 234777-46-9P 234777-47-0P
234777-48-1P 234777-49-2P 234777-50-5P 234777-51-6P 234777-52-7P
234777-53-8P 234777-54-9P 234777-55-0P 234777-56-1P 234777-57-2P
234777-58-3P 234777-59-4P 234777-60-7P 234777-61-8P 234777-62-9P
234777-63-0P 234777-64-1P 234777-65-2P 234777-66-3P 234777-67-4P
234777-68-5P 234777-69-6P 234777-70-9P 234777-71-0P 234777-72-1P
234777-73-2P 234777-74-3P 234777-75-4P 234777-76-5P 234777-77-6P
234777-78-7P 234777-79-8P 234777-80-1P 234777-81-2P 234777-82-3P
234777-83-4P 234777-84-5P 234777-85-6P 234777-86-7P 234777-87-8P
234777-88-9P 234777-89-0P 234777-90-3P 234777-91-4P 234777-92-5P
234777-93-6P 234777-94-7P 234777-95-8P 234777-96-9P 234777-97-0P
234777-98-1P 234777-99-2P 234778-00-8P 234778-01-9P 234778-02-0P
234778-03-1P 234778-04-2P 234778-05-3P 234778-06-4P 234778-07-5P
234778-08-6P 234778-09-7P 234778-10-0P 234778-11-1P 234778-12-2P
234778-13-3P 234778-14-4P 234778-15-5P 234778-16-6P 234778-17-7P
234778-18-8P 234778-19-9P 234778-20-2P 234778-21-3P 234778-22-4P
234778-23-5P 234778-24-6P 234778-25-7P 234778-26-8P 234778-27-9P
234778-28-0P 234778-29-1P 234778-30-4P 234778-31-5P 234778-32-6P
234778-33-7P 234778-34-8P 234778-35-9P 234778-36-0P 234778-37-1P
234778-38-2P 234778-39-3P 234778-40-6P 234778-41-7P 234778-42-8P
234778-43-9P 234778-44-0P 234778-45-1P 234778-46-2P 234778-47-3P
234778-48-4P 234778-49-5P 234778-50-8P 234778-51-9P 234778-52-0P
235083-80-4P 261966-75-0P 262297-98-3P 267233-42-1P 267233-43-2P
267233-44-3P 267233-45-4P 267233-46-5P 267233-47-6P 267233-48-7P
267233-49-8P 267233-50-1P 267233-51-2P 267233-52-3P 267233-53-4P
267233-54-5P 267233-55-6P 267233-56-7P 267233-57-8P 267233-59-0P
267233-60-3P 267233-61-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compound; preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

RE.CNT 68 THERE ARE 68 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

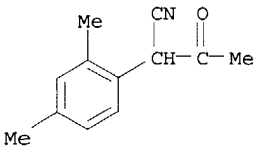
(1) Anon; JP 4211753 1967
(2) Anon; JP 6157587 1986
(3) Anon; EP 0269859 1988 HCAPLUS
(4) Anon; EP 0300688 1989 HCAPLUS
(5) Anon; EP 0373891 1989 HCAPLUS
(6) Anon; EP 0374448 1990 HCAPLUS
(7) Anon; EP 0395144 1990 HCAPLUS
(8) Anon; EP 0455545 1991 HCAPLUS
(9) Anon; EP 0503099 1992 HCAPLUS
(10) Anon; DE 4243279 1992 HCAPLUS
(11) Anon; WO 9210098 1992 HCAPLUS
(12) Anon; WO 9220642 1992 HCAPLUS
(13) Anon; EP 0521622 1993 HCAPLUS
(14) Anon; EP 0531901 1993 HCAPLUS
(15) Anon; EP 0576350 1993 HCAPLUS
(16) Anon; EP 0591528 1994 HCAPLUS
(17) Anon; EP 0594149 1994 HCAPLUS
(18) Anon; WO 9409017 1994 HCAPLUS
(19) Anon; WO 9413643 1994 HCAPLUS
(20) Anon; WO 9413644 1994 HCAPLUS
(21) Anon; WO 9413661 1994 HCAPLUS

(22) Anon; WO 9413676 1994 HCAPLUS
(23) Anon; WO 9413677 1994 HCAPLUS
(24) Anon; EP 0662477 1995 HCAPLUS
(25) Anon; EP 0714898 1995 HCAPLUS
(26) Anon; WO 9500507 1995 HCAPLUS
(27) Anon; WO 9511880 1995 HCAPLUS
(28) Anon; WO 9532710 1995 HCAPLUS
(29) Anon; WO 9533727 1995 HCAPLUS
(30) Anon; WO 9533750 1995 HCAPLUS
(31) Anon; WO 9534563 1995 HCAPLUS
(32) Anon; EP 0729758 1996 HCAPLUS
(33) Anon; WO 9535298 1996 HCAPLUS
(34) Anon; WO 9619452 1996 HCAPLUS
(35) Anon; WO 9623783 1996 HCAPLUS
(36) Anon; WO 9635689 1996 HCAPLUS
(37) Anon; WO 9639388 1996 HCAPLUS
(38) Anon; WO 9639400 1996 HCAPLUS
(39) Anon; EP 0773023 1997 HCAPLUS
(40) Anon; EP 0778277 1997 HCAPLUS
(41) Anon; EP 0812831 1997 HCAPLUS
(42) Anon; WO 9700868 1997 HCAPLUS
(43) Anon; WO 9714684 1997 HCAPLUS
(44) Anon; WO 9729109 1997 HCAPLUS
(45) Anon; WO 9729110 1997 HCAPLUS
(46) Anon; WO 9808821 1998 HCAPLUS
(47) Anon; WO 9808846 1998 HCAPLUS
(48) Anon; WO 9808847 1998 HCAPLUS
(49) Bantick; US 5428044 1995 HCAPLUS
(50) Barker; US 5089499 1992 HCAPLUS
(51) Britton; Life Sciences 1982, V31, P363 HCAPLUS
(52) Britton; Psychopharmacology 1988, V94, P306 HCAPLUS
(53) Bussler; US 5484760 1996 HCAPLUS
(54) Courtemanche; US 5464847 1995 HCAPLUS
(55) Eicken; US 4567263 1986 HCAPLUS
(56) Hashimoto; US 5137887 1992 HCAPLUS
(57) Himmelsbach; US 5463071 1995 HCAPLUS
(58) Himmler; US 4909647 1991
(59) Kruger; US 4892576 1990 HCAPLUS
(60) Nugent; US 5397774 1995 HCAPLUS
(61) O'Brien; US 3910907 1975 HCAPLUS
(62) Rooney; US 3995039 1976 HCAPLUS
(63) Schonafinger; US 5486531 1996 HCAPLUS
(64) Springer; US 3920652 1975 HCAPLUS
(65) Springer; US 4021556 1977 HCAPLUS
(66) Vinogradoff; US 4997940 1991 HCAPLUS
(67) Weinheim; Arch Pharm 1987, V320, P487
(68) Yuan; US 5723608 1998 HCAPLUS

IT **202580-61-8P**, 1-Cyano-1-(2,4-dimethylphenyl)propan-2-one
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(intermediate; preparation of azolo-fused triazines and pyrimidines as CRF antagonists)

RN 202580-61-8 HCAPLUS

CN Benzeneacetonitrile, .alpha.-acetyl-2,4-dimethyl- (9CI) (CA INDEX NAME)



L28 ANSWER 8 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1999:152295 HCAPLUS

DN 130:209711

ED Entered STN: 09 Mar 1999

TI Preparation of phenyl-spiro(cycloalkyl ethers) as tachykinin receptor antagonists

IN Caldwell, Charles G.; Chiang, Yuan-ching; Dorn, Conrad; Finke, Paul; Hale, Jeffrey; Maccoss, Malcolm; Mills, Sander; Robichaud, Albert

PA Merck and Co., Inc., USA

SO U.S., 98 pp.
CODEN: USXXAM

DT **Patent**
LA English
IC ICM A61K031-36
ICS C07D285-04; C07D307-94; C07D311-96
NCL 514337000
CC 28-13 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5877191	A	19990302	US 1997-955898	19971022 <--
PRAI	US 1997-955898		19971022 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 5877191	ICM	A61K031-36
	ICS	C07D285-04; C07D307-94; C07D311-96
	NCL	514337000

OS MARPAT 130:209711
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention is directed to certain novel compds. represented by structural formula [I; R3 is selected from hydrogen, C1-8 alkyl, R4, R4-substituted C1-6 alkyl; R4 is hydroxy, C1-6 alkoxy, phenyl-C1-3 alkoxy, Ph, cyano, halo, (un)substituted NH2, heterocyclyl, (un)substituted CO2H, etc.; R6, R7, and R8 are selected from hydrogen, C1-6 alkyl, halo, (un)substituted C1-6 alkyl, HO, cyano, CF3, CF3O, OCF2H, OCFH2, NO2, SH, C1-6 alkylthio, (un)substituted CO2H or NH2, heterocyclyl, C1-6 alkylheterocyclyl, etc.; R11, R12, and R13 are selected from hydrogen, (un)substituted C1-6 alkyl, halo, cyano, CF3, NO2, HO, C1-6 alkoxy, acyl, (un)substituted CO2H or NH2, etc.; m is an integer of 1 or 2; n is an integer of 0, 1, or 2]. A method for antagonizing the effect of substance P at its receptor site or for the blockade of neurokinin-1 receptors in a mammal comprises the administration to the mammal of the above compound in an amount that is effective for antagonizing the effect of substance P at its receptor site or for the blockade of neurokinin-1 receptors in the mammal. The invention is also concerned with pharmaceutical formulations comprising these novel compds. as active ingredients and the use of the novel compds. and their formulations in the treatment of certain disorders. The compds. of this invention are useful in the treatment of inflammatory diseases, pain or migraine, asthma, and emesis (no data). Thus, Me [5(RS),6(SR),7(SR)]-6-(4-fluorophenyl)-3-(trimethylstannyl)-1-oxaspiro[4,4]hon-3-ene-7-carboxylate was coupled with 3-bromo-4-(5-(trifluoromethyl)tetrazol-1-yl)anisole in the presence of tetrakis(triphenylphosphine)palladium(0) in dioxane at 100.degree. for 1.5 h to give the title compound, Me 5-((5-(trifluoromethyl)tetrazol-1-yl)phenyl)-1-oxaspiro[4.4]nonane-7-carboxylate derivative (II).

ST phenyl spiro cycloalkyl ether prepn tachykinin receptor antagonist; substance P receptor antagonist; neurokinin 1 receptor blocker; inflammatory disease treatment oxaspirononane; pain treatment oxaspirononane; migraine treatment oxaspirononane; asthma treatment oxaspirononane; emesis treatment oxaspirononane; tetrazolylphenyloxaspirononane prepn tachykinin receptor antagonist; oxaspirononane tetrazolyl phenyl prepn tachykinin receptor antagonist

IT Tachykinin receptors
(NK1 antagonists; preparation of phenyl-spiro(cycloalkyl ethers) as tachykinin receptor antagonists for treatment of diseases)

IT Tachykinin receptors
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(antagonists; preparation of phenyl-spiro(cycloalkyl ethers) as tachykinin receptor antagonists for treatment of diseases)

IT Headache
(migraine; preparation of phenyl-spiro(cycloalkyl ethers) as tachykinin receptor antagonists for treatment of diseases)

IT Analgesics
Antiasthmatics
Antiemetics
(preparation of phenyl-spiro(cycloalkyl ethers) as tachykinin receptor antagonists for treatment of diseases)

IT 33507-63-0, Substance P

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(preparation of phenyl-spiro(cycloalkyl ethers) as tachykinin receptor antagonists for treatment of diseases)

IT 50-00-0, Formaldehyde, reactions 57-14-7, 1,1-Dimethylhydrazine 74-88-4, Iodomethane, reactions 75-16-1, Methylmagnesium bromide 75-30-9, 2-Iodopropane 79-24-3, Nitroethane 99-89-8, 4-Isopropylphenol 100-51-6, Benzyl alcohol, reactions 100-52-7, Benzaldehyde, reactions 103-71-9, Phenyl isocyanate, reactions 105-56-6, Ethyl cyanoacetate 108-24-7 110-13-4, 2,5-Hexanedione 110-91-8, Morpholine, reactions 123-75-1, Pyrrolidine, reactions 328-93-8, 2,5-Bis-trifluoromethylaniline 334-88-3, Diazomethane 402-10-8, 2-Bromo-4-(trifluoromethyl)anisole 407-25-0, Trifluoroacetic anhydride 459-57-4, 4-Fluorobenzaldehyde 460-08-2, 2-Fluoroethylamine hydrochloride 623-71-2, Ethyl .beta.-chloropropionate 645-36-3, Aminoacetaldehyde diethyl acetal 661-69-8, Hexamethylditin 828-27-3, 4-Trifluoromethoxyphenol 1427-07-2, 3-Fluoro-4-methylnitrobenzene 1515-78-2, 1-Phenyl-1,3-butadiene 1544-85-0, 2,2-Difluoro-5-aminobenzodioxole 2627-86-3, (S)-(-)-.alpha.-Methylbenzyl amine 2967-66-0, Methyl 4-(trifluoromethyl)benzoate 3886-69-9, (R)-.alpha.-Methylbenzyl amine 4009-98-7, (Methoxymethyl)triphenylphosphonium chloride 5197-28-4, 2-Bromo-4-nitroanisole 5470-11-1, Hydroxylamine hydrochloride 6423-74-1, 3-Bromo-4-isopropoxybenzonitrile 7051-34-5, Bromomethylcyclopropane 7143-01-3, Methanesulfonic anhydride 13296-94-1, 2-Bromo-4-nitroaniline 16911-89-0, Phenyl chlorodithioformate 18962-05-5, 4-Isopropoxybenzaldehyde 24424-99-5, Di-tert-butyl dicarbonate 26386-88-9, Diphenylphosphoryl azide 34841-06-0, 3-Bromo-4-methoxybenzaldehyde 44637-25-4, Trifluoroacetohydroximoyl bromide 69739-34-0, tert-Butyldimethylsilyl triflate 80522-42-5, Triisopropylsilyl triflate 81107-97-3, 2-Bromo-4-(trifluoromethyl)phenol 99583-51-4, 3-Acetoxy-2-[(trimethylstannyl)methyl]-1-propene 145100-51-2 191602-55-8 200956-54-3, 2-Bromo-1-isopropoxy-4-(trifluoromethyl)benzene 207109-42-0 207111-02-2 207111-06-6, N-(3-Bromo-4-(methylthio)phenyl)-2,2,2-trifluoroacetamide 220982-78-5 220982-79-6 220982-80-9 220982-81-0 220982-82-1 220982-83-2 220982-84-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of phenyl-spiro(cycloalkyl ethers) as tachykinin receptor antagonists for treatment of diseases)

IT 2252-62-2P 7617-93-8P, 2,5-Bis-trifluoromethylbromobenzene 19056-41-8P 19432-27-0P, 2-Bromo-4-isopropylphenol 20735-01-7P 20901-65-9P 31558-30-2P 32445-99-1P, 4-Isopropyl-1-(trifluoromethyl)benzene 32990-21-9P, Trifluoroacetonitrile oxide 93484-84-5P 190269-55-7P 190269-57-9P 190269-59-1P 190269-60-4P 190269-69-3P 190269-71-7P 190269-73-9P 190269-75-1P 190269-76-2P 190269-78-4P 190269-79-5P 190269-82-0P 190269-90-0P 190271-11-5P 190271-13-7P 191602-40-1P, 2-Bromo-4-(trifluoroacetamido)anisole 191602-41-2P, 2-Bromo-4-(5-(trifluoromethyl)-1H-tetrazol-1-yl)anisole 191602-56-9P 191602-66-1P 191602-84-3P, 3-Bromo-4-isopropoxybenzaldehyde 200956-13-4P, 2-Bromo-4-(trifluoromethoxy)phenol 200956-14-5P, 2-Bromo-4-(trifluoromethoxy)anisole 206759-09-3P 207110-12-1P 207110-30-3P, 1-Cyclopropylmethoxy-2-bromo-4-(trifluoromethoxy)benzene 207110-31-4P 207110-34-7P, 3-Bromo-5-fluoro-4-methyl-1-nitrobenzene 207110-35-8P, 3-Bromo-5-fluoro-4-methylaniline 207110-36-9P, 3-Bromo-5-fluoro-4-methyltrifluoroacetanilide 207110-37-0P 207110-38-1P, 2-Bromo-1-methoxy-4-(2-methoxyvinyl)benzene **207110-39-2P** **207110-40-5P**, 4-(3-Bromo-4-methoxyphenyl)-3-methylisoxazole 207110-41-6P, 1-(3-Bromo-4-methoxyphenyl)-2,5-dimethylpyrrole 207110-43-8P 207110-45-0P, 4-(3-Bromo-4-methoxyphenyl)-3-methylpyrazole 207110-46-1P, 1-(tert-Butoxycarbonyl)-4-(3-bromo-4-methoxyphenyl)-3-methylpyrazole 207110-47-2P 207110-48-3P 207110-49-4P 207110-52-9P 207110-53-0P 207110-54-1P 207110-55-2P 207110-56-3P 207110-57-4P 207110-58-5P 207110-59-6P 207110-60-9P 207110-61-0P 207110-62-1P 207110-63-2P 207110-67-6P 207110-69-8P 207110-70-1P 207110-71-2P 207110-72-3P 207110-73-4P 207110-74-5P 207110-75-6P 207110-76-7P 207110-77-8P 207110-78-9P 207110-79-0P 207110-80-3P, 2,2-Difluoro-5-(trifluoroacetamide)benzodioxole 207110-82-5P 207110-83-6P 207110-84-7P 207110-85-8P 207110-86-9P **207110-89-2P** 207110-90-5P, 3-(3-Bromo-4-methoxyphenyl)pentane-2,4-dione **207110-91-6P** 207110-92-7P 207110-93-8P 207110-94-9P 207110-95-0P 207110-96-1P 207110-97-2P, 2-Bromo-4-isopropyl-1-(trifluoromethoxy)benzene 207110-98-3P **207111-09-9P** 207111-10-2P 207111-11-3P, 2-Bromo-1-isopropyl-4-(trifluoromethyl)benzene 207111-96-4P 220982-33-2P 220982-34-3P 220982-46-7P 220982-48-9P 220982-49-0P 220982-51-4P 220982-53-6P 220982-55-8P 220982-56-9P 220982-57-0P 220982-58-1P 220982-59-2P

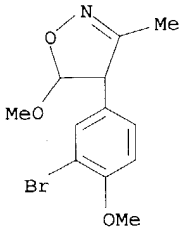
220982-60-5P 220982-61-6P 220982-62-7P 220982-63-8P 220982-64-9P
220982-65-0P 220982-66-1P 220982-67-2P 220982-68-3P 220982-69-4P
220982-70-7P 220982-71-8P 220982-72-9P 220982-74-1P,
2,2-Difluoro-4-bromo-5-(trifluoroacetamide)benzodioxole 220982-75-2P
220982-76-3P, 4-(3-Bromo-4-methoxyphenyl)-3-
(trifluoromethyl)isoxazole 220982-77-4P, 3-(3-Bromo-4-isopropoxyphenyl)-
1,3-pentane-2,4-dione
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP**
(Preparation); RACT (Reactant or reagent)
(preparation of phenyl-spiro(cycloalkyl ethers) as tachykinin receptor
antagonists for treatment of diseases)

IT 206759-01-5P 207108-54-1P 207108-64-3P 207108-69-8P 207108-75-6P
207109-98-6P 207110-00-7P 207110-02-9P 207110-03-0P 207110-05-2P
207110-06-3P 207110-07-4P 207110-24-5P 207110-27-8P 207111-31-7P
207111-35-1P 207111-37-3P 207111-53-3P 207111-90-8P 220982-31-0P
RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent);
USES (Uses)
(preparation of phenyl-spiro(cycloalkyl ethers) as tachykinin receptor
antagonists for treatment of diseases)

IT 207108-55-2P 207108-56-3P 207108-57-4P 207108-58-5P 207108-59-6P
207108-60-9P 207108-61-0P 207108-62-1P 207108-63-2P 207108-65-4P
207108-66-5P **207108-67-6P** 207108-68-7P 207108-70-1P
207108-71-2P 207108-72-3P 207108-73-4P 207108-74-5P 207108-77-8P
207108-78-9P 207108-79-0P 207108-80-3P 207108-81-4P 207108-82-5P
207108-83-6P 207108-84-7P 207108-85-8P 207108-86-9P 207108-87-0P
207108-88-1P 207108-89-2P 207108-90-5P 207108-91-6P 207108-92-7P
207108-93-8P 207108-94-9P 207108-95-0P 207108-96-1P 207108-98-3P
207108-99-4P 207109-00-0P 207109-01-1P 207109-02-2P 207109-03-3P
207109-04-4P 207109-05-5P 207109-06-6P 207109-08-8P 207109-10-2P
207109-13-5P 207109-14-6P 207109-21-5P 207109-22-6P 207109-23-7P
207109-24-8P 207109-25-9P 207109-26-0P 207109-27-1P 207109-28-2P
207109-29-3P 207109-30-6P 207109-31-7P 207109-32-8P 207109-40-8P
207109-45-3P 207109-46-4P 207109-52-2P 207109-53-3P 207109-54-4P
207109-59-9P 207109-63-5P 207109-66-8P 207109-67-9P 207109-68-0P
207109-69-1P 207109-74-8P 207109-75-9P 207109-76-0P 207109-77-1P
207109-80-6P 207109-81-7P 207109-82-8P 207109-83-9P 207109-84-0P
207109-85-1P 207109-86-2P 207109-87-3P 207109-89-5P 207109-90-8P
207109-91-9P 207109-92-0P 207109-93-1P 207109-94-2P 207109-97-5P
207109-99-7P 207110-04-1P 207110-08-5P 207110-09-6P 207110-10-9P
207110-13-2P 207110-14-3P 207110-16-5P **207110-18-7P**
207110-19-8P 207110-20-1P 207110-21-2P 207110-22-3P
207110-23-4P 207110-25-6P 207110-26-7P 207110-28-9P 207110-29-0P
207111-01-1P 207111-12-4P 207111-13-5P 207111-19-1P 207111-24-8P
207111-33-9P 207111-39-5P 207111-41-9P 207111-43-1P 207111-47-5P
207111-48-6P 207111-49-7P 207111-51-1P 207111-52-2P 207111-54-4P
207111-56-6P 207111-57-7P 207111-59-9P 207111-60-2P 207111-61-3P
207111-62-4P 207111-63-5P 207111-64-6P 207111-66-8P 207111-67-9P
207111-68-0P 207111-69-1P 207111-70-4P 207111-71-5P 207111-72-6P
207111-73-7P 207111-74-8P 207111-75-9P 207111-77-1P 207111-78-2P
207111-79-3P 207111-80-6P 207111-81-7P 207111-82-8P 207111-83-9P
207111-84-0P 207111-85-1P 207111-86-2P 207111-88-4P 207111-91-9P
207111-93-1P 207111-94-2P 207111-95-3P 220981-83-9P 220981-84-0P
220981-85-1P 220981-86-2P 220981-87-3P 220981-89-5P 220981-90-8P
220981-91-9P 220981-94-2P 220981-95-3P 220981-97-5P 220981-98-6P
220981-99-7P 220982-00-3P 220982-01-4P 220982-02-5P 220982-03-6P
220982-04-7P 220982-05-8P 220982-06-9P 220982-07-0P 220982-11-6P
220982-12-7P 220982-13-8P 220982-15-0P 220982-16-1P 220982-17-2P
220982-18-3P 220982-19-4P 220982-20-7P 220982-21-8P 220982-22-9P
220982-23-0P 220982-24-1P 220982-25-2P 220982-26-3P 220982-27-4P
220982-28-5P 220982-29-6P 220982-30-9P **220982-32-1P**
RL: **SPN (Synthetic preparation)**; THU (Therapeutic use); BIOL
(Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of phenyl-spiro(cycloalkyl ethers) as tachykinin receptor
antagonists for treatment of diseases)

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Anon; WO 9420500 1994 HCAPLUS
(2) Anon; WO 9620197 1996 HCAPLUS
(3) Anon; WO 9714671 1997 HCAPLUS
(4) Anon; WO 9719084 1997 HCAPLUS
(5) Anon; WO 9730055 1997 HCAPLUS
(6) Anon; WO 9730056 1997 HCAPLUS
(7) Anon; WO 9749710 1997 HCAPLUS
(8) Desai; US 5688806 1997 HCAPLUS
(9) Mills; US 5387595 1995 HCAPLUS

IT **207110-39-2P**
RL: **SPN (Synthetic preparation); SPN (Synthetic preparation); PREP (Preparation); PREP (Preparation)**
(preparation of phenyl-spiro(cycloalkyl ethers) as tachykinin receptor antagonists for treatment of diseases)
RN 207110-39-2 HCAPLUS
CN Isoxazole, 4-(3-bromo-4-methoxyphenyl)-4,5-dihydro-5-methoxy-3-methyl- (9CI) (CA INDEX NAME)



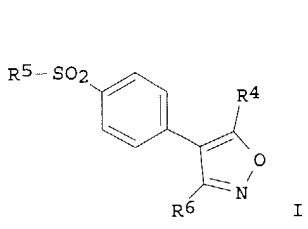
L28 ANSWER 9 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:45215 HCAPLUS
DN 130:110269
ED Entered STN: 22 Jan 1999
TI Preparation of isoxazole compounds as cyclooxygenase inhibitors
IN Talley, John J.
PA G.D. Searle and Co., USA
SO U.S., 52 pp., Cont.-in-part of U.S. 5,633,272.
CODEN: USXXAM
DT **Patent**
LA English
IC ICM C07D261-06
NCL 548247000
CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5859257	A	19990112	US 1996-702417	19960814 <--
	US 5633272	A	19970527	US 1995-473884	19950607 <--
PRAI	US 1995-387680	B2	19950213	<--	
	US 1995-473884	A2	19950607	<--	

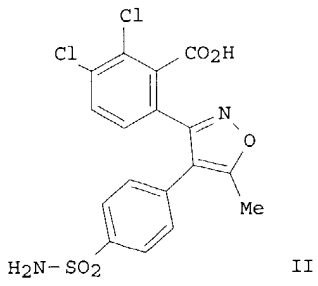
CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 5859257	ICM	C07D261-06
	NCL	548247000

OS CASREACT 130:110269; MARPAT 130:110269
GI



I



II

AB Claimed is a method of preparing title compds. I [R4 = alkyl, etc.; R5 = amino; R6 = (un)substituted phenyl] by treatment of a diphenylethanone derivative with hydroxylamine, treating said oxime with base and an acylating agent to form a diphenylisoxazoline derivative, and forming the (isoxazol-4-yl)benzenesulfonamide by treatment of the isoxazoline with chlorosulfonic acid and ammonia. The title compound II in vitro showed IC50

values of 0.4 .mu.M and > 100 .mu.M against COX-2 and COX-1, resp.

ST isoxazole prepn cyclooxygenase 2 inhibitor; cyclooxygenase 2 inhibitor isoxazole prepn

IT Intestine, disease
(inflammatory; preparation and effect of isoxazole compds. with effect on COX-2)

IT Analgesics
(preparation and effect of isoxazole compds. as cyclooxygenase inhibitors)

IT Alzheimer's disease
Arthritis
(preparation and effect of isoxazole compds. with effect on COX-2)

IT Anti-inflammatory agents
(preparation of isoxazole compds. as cyclooxygenase inhibitors)

IT Intestine, disease
(ulcerative colitis; preparation and effect of isoxazole compds. with effect on COX-2)

IT **181695-72-7P 181695-73-8P 181695-74-9P**
181695-75-0P 181695-76-1P 181695-77-2P
181695-78-3P 181695-79-4P 181695-80-7P
181695-81-8P 181695-82-9P 181695-83-0P
181695-84-1P 181695-85-2P 181695-86-3P
181695-87-4P 181695-88-5P 181695-89-6P
181695-90-9P 181695-91-0P 181695-92-1P
181695-93-2P 181695-94-3P 181695-95-4P
181695-96-5P 181695-97-6P 181695-98-7P
181695-99-8P 181696-00-4P 181696-01-5P
181696-02-6P 181696-03-7P 181696-04-8P
181696-05-9P 181696-06-0P 181696-07-1P
181696-08-2P 181696-09-3P 181696-10-6P 181696-11-7P
181696-12-8P 181696-13-9P 181696-14-0P
181696-15-1P 181696-16-2P 181696-17-3P
181696-18-4P 181696-19-5P 181696-20-8P
181696-21-9P 181696-22-0P 181696-23-1P
181696-24-2P 181696-25-3P 181696-26-4P
181696-27-5P 181696-28-6P 181696-29-7P
181696-30-0P 181696-31-1P 181696-32-2P
181696-33-3P 181696-34-4P 181696-35-5P
181696-36-6P 181696-37-7P 181696-38-8P
181696-39-9P 181696-40-2P 181696-41-3P
181696-42-4P 181696-43-5P 181696-44-6P
181696-45-7P 181696-46-8P 195061-34-8P
219679-53-5P 219679-54-6P 219679-55-7P
219679-56-8P 219679-57-9P **219679-58-0P 219679-59-1P**
219679-60-4P 219679-61-5P 219679-62-6P
219679-63-7P 219679-64-8P 219679-65-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); **IMF (Industrial manufacture)**; **SPN (Synthetic preparation)**; THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of isoxazole compds. as cyclooxygenase inhibitors)

IT 39391-18-9, Cyclooxygenase
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)
(preparation of isoxazole compds. as cyclooxygenase inhibitors)

IT 64-17-5, Ethanol, reactions 71-43-2, Benzene, reactions 75-16-1, Methylmagnesium bromide 75-36-5, Acetyl chloride 79-20-9 98-59-9, Toluenesulfonyl chloride 99-76-3, Methyl 4-hydroxybenzoate 100-39-0, Benzyl bromide 100-52-7, Benzaldehyde, reactions 101-41-7, Methyl phenylacetate 103-79-7, Phenylacetone 103-80-0, Phenylacetyl chloride 103-82-2, Phenylacetic acid, reactions 104-87-0, p-Tolualdehyde 104-88-1, p-Chlorobenzaldehyde, reactions 108-24-7 108-30-5, Succinic anhydride, reactions 108-55-4, Glutaric anhydride 108-89-4 109-72-8, Butyllithium, reactions 110-13-4, Acetonylacetone 123-11-5, 4-Anisaldehyde, reactions 124-38-9, Carbon dioxide, reactions 321-28-8, 2-Fluoroanisole 358-23-6, Trifluoromethanesulfonic anhydride 451-40-1, Desoxybenzoin 459-57-4, 4-Fluorobenzaldehyde 553-90-2, Dimethyl oxalate 587-04-2, 3-Chlorobenzaldehyde 693-03-8, Butylmagnesium bromide 766-51-8, 2-Chloroanisole 925-90-6, Ethylmagnesium bromide 1007-32-5, 1-Phenyl-2-butanone 1122-91-4, 4-Bromobenzaldehyde 1336-21-6, Ammonium hydroxide 1722-69-6, 1,2-Diphenyl-1-buten-3-one 2466-76-4, N-Acetylimidazole 2646-90-4, 2,5-Difluorobenzaldehyde 2893-05-2 2950-43-8, Hydroxylamine O-sulfonic acid 3446-89-7, 4-(Methylthio)benzaldehyde 3795-79-7, Methyl 4-(methylthio)benzoate 4111-54-0, Lithium diisopropylamide 4166-53-4, 3-Methylglutaric anhydride 4206-67-1, Trimethylsilyliodomethane 4480-83-5, 1,4-Dioxane-2,6-dione 5188-07-8, Sodium thiomethoxide

5470-11-1, Hydroxylamine hydrochloride 6287-38-3, 3,4-Dichlorobenzaldehyde 6638-79-5, N,O-Dimethylhydroxylamine hydrochloride 6683-92-7, 1-Phenyl-2-pentanone 7446-09-5, Sulfur dioxide, reactions 7664-41-7, Ammonia, reactions 7677-24-9, Trimethylsilylcyanide 7790-94-5, Chlorosulfonic acid 13528-93-3, Bis(1,2-chlorodimethylsilyl)ethane 16188-55-9, 4-(Methylthio)phenylacetic acid 24424-99-5, Di-tert-butyl dicarbonate 34036-07-2, 3,4-Difluorobenzaldehyde 63327-11-7 88356-92-7 104372-31-8 219679-80-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of isoxazole compds. as cyclooxygenase inhibitors)

IT 325-62-2P 492-38-6P 952-06-7P 1023-17-2P 1529-41-5P 2001-28-7P 2001-29-8P 3475-29-4P 6318-76-9P 6574-99-8P 13721-20-5P 16736-09-7P 16736-13-3P 16737-10-3P 25632-70-6P 25870-62-6P 26306-06-9P 37612-52-5P **37928-17-9P** 62482-45-5P 63954-98-3P **78967-09-6P** 93534-22-6P 104896-80-2P 121411-85-6P 177560-74-6P 177561-49-8P **181696-73-1P** 181696-74-2P **181696-75-3P** **181696-76-4P** **181696-77-5P** **181696-78-6P** **181696-79-7P** 181696-80-0P 181696-82-2P 181696-83-3P **181696-84-4P** 181696-85-5P 181696-86-6P 181696-87-7P **181696-88-8P** **181696-89-9P** 181696-90-2P **181696-91-3P** 181696-92-4P 181696-93-5P **181696-94-6P** 181696-96-8P **181696-97-9P** 181696-98-0P 181697-00-7P 181697-01-8P 181697-02-9P **181697-03-0P** **181697-04-1P** 181697-05-2P 181697-06-3P 181697-07-4P **181697-08-5P** **181697-09-6P** **181697-10-9P** **181697-11-0P** **181697-12-1P** **181697-13-2P** **181697-14-3P** 181697-15-4P 181697-16-5P 181697-17-6P 181697-18-7P **181697-19-8P** 181697-20-1P 181697-21-2P **181697-22-3P** 181697-23-4P 181697-24-5P 181697-25-6P 181697-26-7P **181697-28-9P** 181697-29-0P 181697-30-3P 181697-31-4P **181697-32-5P** **181697-33-6P** 185345-56-6P **219679-66-0P** **219679-67-1P** **219679-68-2P** 219679-69-3P **219679-70-6P** 219679-71-7P 219679-72-8P 219679-73-9P **219679-74-0P** **219679-75-1P** **219679-76-2P** 219679-77-3P **219679-78-4P** 219679-79-5P
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of isoxazole compds. as cyclooxygenase inhibitors)

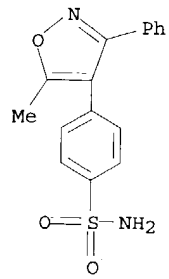
RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Anon; EP 026928 1981 HCAPLUS
(2) Anon; JP 2223568 1990
(3) Anon; JP 4173780 1992
(4) Anon; WO 9219604 1992 HCAPLUS
(5) Anon; EP 549797 1993 HCAPLUS
(6) Anon; AU 9335480 1993 HCAPLUS
(7) Anon; DE 4314966 1994 HCAPLUS
(8) Anon; EP 623603 1994 HCAPLUS
(9) Anon; WO 9417059 1994 HCAPLUS
(10) Anon; WO 9420475 1994 HCAPLUS
(11) Anon; EP 633254 1995 HCAPLUS
(12) Anon; WO 9500501 1995 HCAPLUS
(13) Anon; WO 9512587 1995 HCAPLUS
(14) Anon; WO 9514672 1995 HCAPLUS
(15) Descamps; Bull Soc Chim Belg 1964, V73, P459 HCAPLUS
(16) Hagiwara; US 5310926 1994 HCAPLUS
(17) Suzuki; US 5318970 1994 HCAPLUS
(18) Talley; US 5633272 1997 HCAPLUS
(19) Umezawa; Chem 1963, V36(9), P1150 HCAPLUS
(20) Yamawaki, I; Chem Pharm Bull 1988, V36, P3142 HCAPLUS

IT **181695-72-7P**
RL: BAC (Biological activity or effector, except adverse); **SPN (Synthetic preparation)**; **PREP (Preparation)**; **SPN (Synthetic preparation)**; THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of isoxazole compds. as cyclooxygenase inhibitors)

RN 181695-72-7 HCAPLUS
CN Benzenesulfonamide, 4-(5-methyl-3-phenyl-4-isoxazolyl)- (9CI) (CA INDEX NAME)



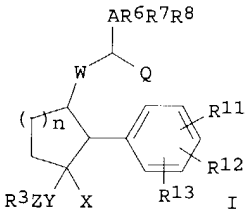
L28 ANSWER 10 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:306975 HCAPLUS
DN 129:15967
ED Entered STN: 25 May 1998
TI Preparation of arylcycloalkanes as tachykinin receptor antagonists.
IN Caldwell, Charles G.; Chen, Ping; Durette, Philippe L.; Finke, Paul; Hale, Jeffrey; Holson, Edward; Kopka, Ihor; Maccoss, Malcolm; Meurer, Laura; Mills, Sander G.; Robichaud, Albert
PA Merck and Co., Inc., USA
SO U.S., 109 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC ICM A61K031-41
ICS C07D257-04; C07D271-10
NCL 514364000
CC 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1, 27, 28
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 5750549	A	19980512	US 1996-730277	19961015 <--
PRAI US 1996-730277		19961015 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 5750549	ICM	A61K031-41
	ICS	C07D257-04; C07D271-10
	NCL	514364000

OS MARPAT 129:15967
GI



AB Title compds. [I; R3 = H, alkoxy, phenylalkoxy, Ph, cyano, halo, amino, (substituted) alkyl, null; R6-R8 = H, alkoxy, halo, (substituted) alkyl, OH, cyano, CF3, NO2, heterocyclyl, etc.; R11-R13 = H, (substituted) alkyl, halo, cyano, CF3, NO2, OH, alkoxy, etc.; A = Ph, benzofuranyl, benzothiophenyl, benzothiazoyl, indolyl, imidazolyl, oxadiazolyl, pyridyl, pyrimidyl, quinolinyl, thiazolyl, thienyl, thiophenyl, dihydrobenzofuranyl; Q = H, alkyl; W = O, NH, alkylimino, NHCO, alkyliminocarbonyl; X = H, alkyl; Y = bond, (substituted) alkyl; Z = NR15, CONR15, SO2NR15, SO2, CO2R15, CH2OR15, null; R15 = H, (substituted) alkyl; n = 1-3; with provisos], were prepared Thus, Me 3(SR)-hydroxy-2(RS)-phenylcyclopentane-1(RS)-carboxylate (preparation given) was treated with 3,5-bis(trifluoromethyl)benzyl bromide and NaH in DMF to give Me 3(SR)-[3,5-bis(trifluoromethyl)phenylmethoxy]-2(RS)-phenylcyclopentane-1(RS)-carboxylate. I showed intrinsic tachykinin receptor antagonist activity in the range 0.05-10 .mu.M.

ST arylcycloalkane prepn tachykinin receptor antagonist; substance P antagonist arylcycloalkane prepn

IT Nerve, disease
(diabetic neuropathy, treatment; preparation of arylcycloalkanes as tachykinin receptor antagonists)

IT Nerve, disease
(neuralgia, treatment; preparation of arylcycloalkanes as tachykinin receptor antagonists)

IT Nerve, disease
(neuropathy, treatment; preparation of arylcycloalkanes as tachykinin receptor antagonists)

IT Nerve, disease
(peripheral neuropathy, treatment; preparation of arylcycloalkanes as tachykinin receptor antagonists)

IT Analgesics
(preparation of arylcycloalkanes as tachykinin receptor antagonists)

IT Cystic fibrosis
(treatment; preparation of arylcycloalkanes as tachykinin receptor antagonists)

IT 33507-63-0P, Substance P 86933-74-6P, Neurokinin A
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(antagonists; preparation of arylcycloalkanes as tachykinin receptor antagonists)

IT 190268-90-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of)

IT

190266-01-4P	190266-02-5P	190266-05-8P	190266-06-9P	190266-07-0P
190266-08-1P	190266-09-2P	190266-10-5P	190266-11-6P	190266-12-7P
190266-13-8P	190266-14-9P	190266-15-0P	190266-16-1P	190266-17-2P
190266-18-3P	190266-19-4P	190266-20-7P	190266-21-8P	190266-22-9P
190266-23-0P	190266-24-1P	190266-25-2P	190266-26-3P	190266-27-4P
190266-28-5P	190266-29-6P	190266-30-9P	190266-31-0P	190266-32-1P
190266-33-2P	190266-35-4P	190266-37-6P	190266-39-8P	190266-41-2P
190266-43-4P	190266-45-6P	190266-46-7P	190266-47-8P	190266-48-9P
190266-49-0P	190266-50-3P	190266-51-4P	190266-53-6P	190266-55-8P
190266-57-0P	190266-58-1P	190266-59-2P	190266-60-5P	190266-61-6P
190266-63-8P	190266-64-9P	190266-65-0P	190266-66-1P	190266-67-2P
190266-68-3P	190266-69-4P	190266-70-7P	190266-71-8P	190266-72-9P
190266-73-0P	190266-74-1P	190266-75-2P	190266-76-3P	190266-77-4P
190266-78-5P	190266-79-6P	190266-80-9P	190266-81-0P	190266-82-1P
190266-83-2P	190266-84-3P	190266-85-4P	190266-86-5P	190266-87-6P
190266-88-7P	190266-89-8P	190266-91-2P	190266-92-3P	190266-93-4P
190266-94-5P	190266-95-6P	190266-96-7P	190266-97-8P	190266-98-9P
190266-99-0P	190267-00-6P	190267-01-7P	190267-02-8P	190267-03-9P
190267-04-0P	190267-05-1P	190267-06-2P	190267-07-3P	190267-08-4P
190267-09-5P	190267-10-8P	190267-11-9P	190267-12-0P	190267-13-1P
190267-14-2P	190267-15-3P	190267-16-4P	190267-17-5P	190267-18-6P
190267-19-7P	190267-20-0P	190267-21-1P	190267-22-2P	190267-23-3P
190267-24-4P	190267-25-5P	190267-26-6P	190267-27-7P	190267-28-8P
190267-29-9P	190267-30-2P	190267-31-3P	190267-32-4P	190267-33-5P
190267-34-6P	190267-35-7P	190267-36-8P	190267-37-9P	190267-38-0P
190267-39-1P	190267-40-4P	190267-41-5P	190267-42-6P	190267-43-7P
190267-44-8P	190267-45-9P	190267-46-0P	190267-47-1P	190267-48-2P
190267-49-3P	190267-50-6P	190267-51-7P	190267-52-8P	190267-53-9P
190267-54-0P	190267-55-1P	190267-56-2P	190267-57-3P	190267-58-4P
190267-59-5P	190267-60-8P	190267-61-9P	190267-62-0P	190267-63-1P
190267-64-2P	190267-65-3P	190267-67-5P	190267-68-6P	190267-69-7P
190267-70-0P	190267-71-1P	190267-72-2P	190267-73-3P	190267-74-4P
190267-75-5P	190267-76-6P	190267-77-7P	190267-78-8P	190267-79-9P
190267-80-2P	190267-81-3P	190267-82-4P	190267-83-5P	190267-84-6P
190267-85-7P	190267-87-9P	190267-89-1P	190267-91-5P	190267-93-7P
190267-95-9P	190267-97-1P	190267-99-3P	190268-03-2P	190268-05-4P
190268-09-8P	190268-13-4P	190268-17-8P	190268-19-0P	190268-21-4P
190268-23-6P	**190268-24-7P**	190268-26-9P	190268-28-1P	
190268-30-5P	190268-32-7P	190268-34-9P	190268-38-3P	190268-40-7P
190268-44-1P	190268-45-2P	190268-46-3P	190268-47-4P	190268-48-5P
190268-49-6P	190268-51-0P	190268-52-1P	190268-53-2P	190268-54-3P
190268-55-4P	190268-56-5P	190268-57-6P	190268-58-7P	190268-60-1P
190268-61-2P	190268-62-3P	190268-63-4P	190268-64-5P	190268-66-7P
190268-68-9P	190268-70-3P	190268-72-5P	190268-74-7P	190268-76-9P
190268-78-1P	190268-80-5P	190268-82-7P	190268-84-9P	190268-86-1P
190268-88-3P	190268-92-9P	190268-97-4P	190269-00-2P	190269-02-4P
190269-05-7P	190269-10-4P	190269-11-5P	190269-12-6P	190269-15-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); **SPN (Synthetic preparation)**; THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of arylcycloalkanes as tachykinin receptor antagonists)

IT 190269-17-1P 190269-19-3P 190269-21-7P 190269-22-8P 190269-23-9P
190269-25-1P 190269-27-3P 190269-29-5P 190269-34-2P 190269-37-5P
190269-40-0P 190269-41-1P 190269-42-2P 190269-46-6P 190269-50-2P
190269-51-3P 190269-52-4P 190269-53-5P 190271-20-6P 190402-06-3P
207729-29-1P 207729-32-6P 207729-34-8P 207729-36-0P 207729-38-2P
207729-45-1P 207729-54-2P 207729-55-3P 207730-34-5P 207730-35-6P
207730-36-7P 207730-37-8P 207730-55-0P 207730-56-1P 207730-57-2P
207730-70-9P 207730-71-0P 207730-73-2P 207730-74-3P 207730-83-4P
207730-89-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of arylcycloalkanes as tachykinin receptor antagonists)

IT 70-23-5, Ethyl bromopyruvate 75-16-1, Methylmagnesium bromide 75-30-9, 2-Iodopropane 79-22-1, Methyl chloroformate 79-44-7, Dimethylcarbamoyl chloride 100-52-7, Benzaldehyde, reactions 105-56-6, Ethyl cyanoacetate 109-04-6, 2-Bromopyridine 123-75-1, Pyrrolidine, reactions 144-48-9, Iodoacetamide 288-32-4, Imidazole, reactions 459-57-4, 4-Fluorobenzaldehyde 609-71-2, 2-Hydroxy-3-carboxypyridine 624-83-9, Methyl isocyanate 624-84-0, Formic hydrazide 626-55-1, 3-Bromopyridine 635-21-2, 2-Chloro-5-aminobenzoic acid 785-56-8, 3,5-Bis(trifluoromethyl)benzoyl chloride 874-60-2, 4-Methylbenzoyl chloride 1066-54-2, Trimethylsilylacetylene 1515-78-2, 1-Phenyl-1,3-butadiene 1761-61-1, 5-Bromosalicylaldehyde 1765-93-1, 4-Fluorobenzeneboronic acid 1779-49-3, Methyltriphenylphosphonium bromide 2362-61-0 2393-23-9, 4-Methoxybenzylamine 2941-72-2, 6-Methoxy-2-methylbenzothiazole 3034-55-7, 5-Bromothiazole 4405-13-4, Glyoxal trimer dihydrate 4892-02-8, Methyl thiosalicylate 5292-43-3, tert-Butyl bromoacetate 6165-68-0, Thiophene-2-boronic acid 6482-24-2, 2-Methoxyethyl bromide 6959-48-4, 3-Picolyl chloride hydrochloride 7252-83-7, Bromoacetaldehyde dimethyl acetal 7531-52-4, L-Prolineamide 14006-51-0, 3-Methoxybenzo[b]thiophene-2-carboxaldehyde 25016-01-7 30071-93-3 32247-96-4, 3,5-Bis(trifluoromethyl)benzyl bromide 34259-99-9, 4-Bromothiazole 35134-07-7, 3-Methoxythiophene-2-carboxaldehyde 36805-97-7, N,N-Dimethylformamide di-tert-butyl acetal 67868-79-5 68236-21-5 72479-05-1 82069-74-7, 3-Methoxythiophene-4-carboxaldehyde 89378-75-6 90719-27-0 92623-00-2 98273-19-9, 2-Methoxycarbonyl-4,6-dichloropyridine 119795-13-0 121124-97-8, 3-Formyl-4-methoxyphenylboronic acid 145742-65-0 155742-64-6 163257-18-9 168266-93-1 168267-02-5 168267-11-6 170682-36-7 170729-89-2 172480-83-0 175205-84-2 175277-50-6 180574-24-7 190269-95-5 190270-88-3 190270-91-8, 6-Methoxy-2-methylbenzothiazole-7-carboxaldehyde 190271-57-9 190271-65-9 190271-66-0 190271-67-1 190271-68-2 190271-69-3 190271-70-6 190271-71-7 190271-72-8, 3-Methoxyquinolin-2-carboxaldehyde 190271-73-9 190271-74-0 190271-75-1 190271-77-3 190271-78-4, 5-Methoxycarbonyl-2-isopropoxybenzaldehyde 190271-79-5, 5-Aminocarbonyl-2-isopropoxybenzaldehyde 190271-80-8 190271-81-9 190271-82-0 190271-83-1 190271-84-2 207730-03-8 207730-05-0 207730-06-1 207730-07-2 207730-08-3 207730-09-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of arylcycloalkanes as tachykinin receptor antagonists)

IT 368-63-8P 3704-28-7P, Methyl 2-methylthiobenzoate 6854-07-5P, 2-Hydroxy-3-carboxy-5-nitropyridine 33384-77-9P, 2-(Methylthio)benzyl alcohol 38185-19-2P 42122-75-8P 53606-06-7P, 2-(Methylsulfonyl)benzyl bromide 122433-50-5P 122433-51-6P 132683-62-6P, 2-Formyl-4,6-dichloropyridine 138505-25-6P, 5-Bromo-2-isopropoxybenzaldehyde 145742-56-9P 160376-84-1P 163257-19-0P 163257-23-6P 168267-13-8P 190268-01-0P 190268-07-6P 190268-11-2P 190268-15-6P 190268-18-9P 190268-20-3P 190268-22-5P 190269-13-7P 190269-54-6P 190269-55-7P 190269-57-9P 190269-59-1P 190269-60-4P 190269-62-6P 190269-64-8P 190269-66-0P 190269-67-1P 190269-69-3P 190269-71-7P 190269-73-9P 190269-75-1P 190269-76-2P 190269-78-4P 190269-79-5P 190269-81-9P 190269-82-0P 190269-86-4P 190269-88-6P 190269-89-7P 190269-90-0P 190269-91-1P 190269-93-3P 190269-96-6P 190269-97-7P 190269-98-8P 190269-99-9P 190270-00-9P 190270-01-0P 190270-03-2P 190270-04-3P 190270-06-5P 190270-07-6P 190270-09-8P 190270-10-1P 190270-11-2P 190270-12-3P 190270-13-4P 190270-14-5P 190270-15-6P 190270-16-7P 190270-17-8P 190270-18-9P 190270-19-0P 190270-20-3P 190270-21-4P 190270-22-5P 190270-23-6P 190270-24-7P 190270-25-8P 190270-26-9P 190270-32-7P 190270-33-8P

190270-34-9P 190270-45-2P 190270-46-3P 190270-47-4P 190270-48-5P
190270-49-6P 190270-50-9P 190270-51-0P 190270-52-1P 190270-53-2P
190270-54-3P 190270-55-4P 190270-56-5P 190270-57-6P 190270-58-7P
190270-59-8P 190270-60-1P 190270-62-3P 190270-63-4P 190270-64-5P
190270-67-8P 190270-69-0P 190270-71-4P 190270-73-6P 190270-76-9P
190270-78-1P 190270-81-6P 190270-84-9P 190270-85-0P 190270-86-1P
190270-87-2P 190270-89-4P 190270-90-7P 190270-92-9P,
5-Cyano-2-isopropoxybenzaldehyde 190270-93-0P 190270-94-1P
190270-95-2P 190270-96-3P 190270-97-4P 190270-99-6P,
1(S)-Hydroxy-2(S)-phenyl-3(R)-hydroxymethylcyclohexane 190271-00-2P
190271-01-3P 190271-02-4P 190271-03-5P 190271-04-6P 190271-06-8P
190271-07-9P 190271-09-1P 190271-11-5P 190271-13-7P 190271-15-9P
190271-18-2P 190271-19-3P 190271-21-7P 190271-22-8P 190271-24-0P
190271-25-1P 190271-26-2P 190271-27-3P 190271-28-4P 190271-29-5P
190271-30-8P 190271-31-9P 190271-32-0P 190271-33-1P 190271-34-2P
190271-35-3P 190271-36-4P 190271-37-5P 190271-42-2P 190271-43-3P
190271-44-4P 190271-45-5P 190271-46-6P 190271-47-7P 190271-48-8P
190271-49-9P 190271-50-2P 190271-51-3P 190271-52-4P 190271-53-5P
190271-54-6P 190271-55-7P 190271-56-8P 190271-87-5P 190271-89-7P
190332-85-5P 190333-61-0P 206759-09-3P 207729-56-4P 207729-58-6P
207729-59-7P 207729-72-4P 207729-74-6P 207729-75-7P 207729-77-9P
207729-79-1P 207729-84-8P 207729-86-0P 207729-87-1P 207729-88-2P
207729-89-3P 207729-90-6P 207729-91-7P 207729-92-8P 207729-93-9P
207729-94-0P 207729-95-1P 207729-96-2P 207729-97-3P 207729-98-4P
207729-99-5P 207730-00-5P 207730-01-6P 207730-72-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of arylcycloalkanes as tachykinin receptor antagonists)

RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

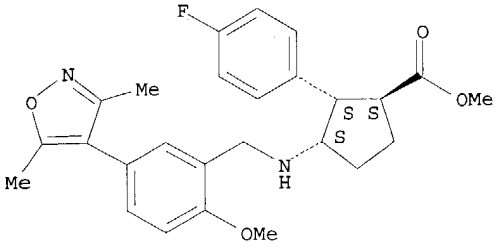
(1) Anon; EP 0142322 1985 HCAPLUS
(2) Anon; EP 0436334 A2 1991 HCAPLUS
(3) Anon; WO 9300331 1993 HCAPLUS
(4) Anon; WO 9400440 1994 HCAPLUS
(5) Anon; WO 9515311 1995 HCAPLUS
(6) Anon; WO 9516679 1995 HCAPLUS
(7) Anon; Chemical Abstracts 1966, V64(8), P12732
(8) Baker; US 5444074 1995 HCAPLUS
(9) Baker; US 5496833 1996 HCAPLUS
(10) Braus; US 3574165 1971 HCAPLUS
(11) Dorn; US 5512570 1996 HCAPLUS
(12) Mills; US 5387595 1995 HCAPLUS
(13) Miura; US 4755617 1988 HCAPLUS
(14) Seward; US 5561130 1996 HCAPLUS
(15) Williams; US 5459270 1995 HCAPLUS

IT **190268-23-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); **SPN (Synthetic preparation)**; THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of arylcycloalkanes as tachykinin receptor antagonists)

RN 190268-23-6 HCAPLUS

CN Cyclopentanecarboxylic acid, 3-[[[5-(3,5-dimethyl-4-isoxazolyl)-2-methoxyphenyl]methyl]amino]-2-(4-fluorophenyl)-, methyl ester, monohydrochloride, (1R,2R,3R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



● HCl

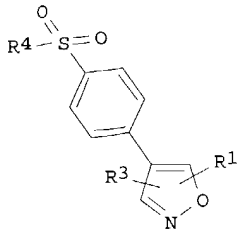
L28 ANSWER 11 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:372654 HCAPLUS
DN 127:65756
ED Entered STN: 14 Jun 1997
TI Preparation of substituted isoxazoles for the treatment of inflammation
IN Talley, John J.; Brown, David L.; Nagarajan, Srinivasan; Carter, Jeffery S.; Weier, Richard M.; Stealey, Michael A.; Collins, Paul W.; Rogers, Roland S.; Seibert, Karen
PA USA
SO U.S., 28 pp., Cont.-in-part of U.S. Ser. No. 387,680, abandoned.
CODEN: USXXAM
DT **Patent**
LA English
IC ICM C07D261-06
ICS C07D261-10; C07D261-12; C07D261-14; A61K031-42
NCL 514378000
CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5633272	A	19970527	US 1995-473884	19950607 <--
	CA 2212836	AA	19960822	CA 1996-2212836	19960212 <--
	CA 2212836	C	20030812		
	WO 9625405	A1	19960822	WO 1996-US1869	19960212 <--
	W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI				
	RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR				
	AU 9648671	A1	19960904	AU 1996-48671	19960212 <--
	AU 699593	B2	19981210		
	BR 9607035	A	19971104	BR 1996-7035	19960212 <--
	EP 809636	A1	19971203	EP 1996-904614	19960212 <--
	EP 809636	B1	20020904		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE				
	CN 1181075	A	19980506	CN 1996-193240	19960212 <--
	CN 1107058	B	20030430		
	JP 11503722	T2	19990330	JP 1996-525057	19960212 <--
	JP 3267300	B2	20020318		
	JP 2002179656	A2	20020626	JP 2001-326343	19960212 <--
	EP 1223167	A2	20020717	EP 2002-3253	19960212 <--
	EP 1223167	A3	20020807		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE				
	AT 223390	E	20020915	AT 1996-904614	19960212 <--
	PT 809636	T	20021231	PT 1996-904614	19960212 <--
	RU 2200158	C2	20030310	RU 1997-115452	19960212 <--
	ES 2183935	T3	20030401	ES 1996-904614	19960212 <--
	PL 185510	B1	20030530	PL 1996-321814	19960212 <--
	PL 185544	B1	20030530	PL 1996-351239	19960212 <--
	CZ 293211	B6	20040317	CZ 1997-2546	19960212 <--
	ZA 9601150	A	19970212	ZA 1996-1150	19960213 <--
	TW 449587	B	20010811	TW 1996-85109684	19960809 <--
	US 5859257	A	19990112	US 1996-702417	19960814 <--
	US 5985902	A	19991116	US 1997-801768	19970218 <--
	FI 9703292	A	19970811	FI 1997-3292	19970811 <--
	NO 9703711	A	19971006	NO 1997-3711	19970812 <--
	CN 1442139	A	20030917	CN 2003-107042	20030228 <--
PRAI	US 1995-387680	B2	19950213 <--		
	US 1995-473884	A	19950607 <--		
	EP 1996-904614	A3	19960212 <--		
	JP 1996-525057	A3	19960212 <--		
	WO 1996-US1869	W	19960212 <--		

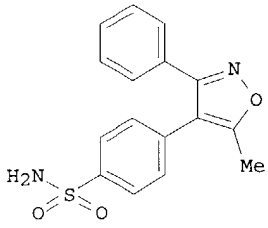
CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 5633272	ICM	C07D261-06
	ICS	C07D261-10; C07D261-12; C07D261-14; A61K031-42
	NCL	514378000

OS MARPAT 127:65756
GI



I



II

AB The title compds. [I; R1 = alkyl, carboxyalkyl, alkoxyalkyl, etc.; R3 = (un)substituted cycloalkyl, cycloalkenyl, aryl; R4 = lower alkyl, OH, NH2], useful in treatment of inflammation and inflammation-associated disorders such as arthritis, pain, and fever, were prepared Thus, treatment of desoxybenzoin oxime with BuLi/hexanes in THF followed by addition of Ac2O, reaction of the resulting 3,4-diphenyl-4-hydro-5-hydroxy-5-methylisoxazole with ClSO3H, and treatment of the intermediate with saturated NH4OH solution afforded 30% II which showed ID50 of < 0.1 .mu.M against COX-2.

ST isoxazole prepn antiinflammatory; antiarthritic isoxazole prepn; analgesic isoxazole prepn; antipyretic isoxazole prepn; cyclooxygenase inhibitor isoxazole prepn

IT Analgesics
Anti-inflammatory agents
Antiarthritics
Antipyretics
(preparation of substituted isoxazoles for the treatment of inflammation)

IT 39391-18-9
RL: BPR (Biological process); BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study); PROC (Process)
(COX-2 inhibitors; preparation of substituted isoxazoles for the treatment of inflammation)

IT **181695-72-7P 181695-81-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); **SPN (Synthetic preparation)**; THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; RACT (Reactant or reagent); USES (Uses)
(preparation of substituted isoxazoles for the treatment of inflammation)

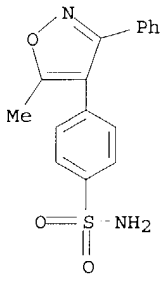
IT **181695-73-8P 181695-74-9P 181695-75-0P**
181695-76-1P 181695-78-3P 181695-79-4P
181695-80-7P 181695-82-9P 181695-83-0P
181695-84-1P 181696-24-2P 181696-25-3P
181696-26-4P 181696-27-5P 181696-28-6P
181696-29-7P 181696-30-0P 181696-31-1P
181696-32-2P 181696-33-3P 181696-34-4P
181696-35-5P 181696-36-6P 181696-37-7P
181696-38-8P 181696-39-9P 181696-40-2P
181696-41-3P 181696-42-4P 181696-43-5P
181696-44-6P 181696-45-7P 191421-97-3P
191421-98-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); **SPN (Synthetic preparation)**; THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of substituted isoxazoles for the treatment of inflammation)

IT 71-43-2, Benzene, reactions 103-80-0, Phenylacetyl chloride 108-30-5, Succinic anhydride, reactions 321-28-8, 2-Fluoroanisole 451-40-1, Desoxybenzoin 766-51-8, 2-Chloroanisole 1722-69-6, 1,2-Diphenyl-1-buten-3-one 3446-89-7, 4-Methylthiobenzaldehyde 63327-11-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of substituted isoxazoles for the treatment of inflammation)

IT 325-62-2P 952-06-7P 3475-29-4P 13721-20-5P, 3-Chloro-4-methoxyphenylacetic acid 25632-70-6P 37612-52-5P **37928-17-9P**
78967-09-6P 177560-74-6P **181696-73-1P** 181696-74-2P
181696-75-3P 181696-76-4P 181696-77-5P
181696-78-6P 181696-80-0P **181696-81-1P** 181696-82-2P
181696-83-3P **181696-84-4P** 181696-85-5P 181696-86-6P
181696-87-7P **181696-89-9P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of substituted isoxazoles for the treatment of inflammation)

IT **181695-72-7P**

RL: BAC (Biological activity or effector, except adverse); **SPN (Synthetic preparation)**; **PREP (Preparation)**; **SPN (Synthetic preparation)**; THU (Therapeutic use); **PREP (Preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent); USES (Uses)
(preparation of substituted isoxazoles for the treatment of inflammation)
RN 181695-72-7 HCAPLUS
CN Benzenesulfonamide, 4-(5-methyl-3-phenyl-4-isoxazolyl)- (9CI) (CA INDEX NAME)



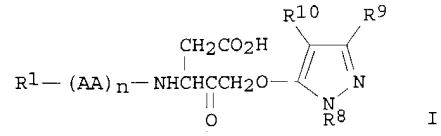
L28 ANSWER 12 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:70248 HCAPLUS
DN 126:144549
ED Entered STN: 31 Jan 1997
TI Preparation of peptidyl heteroaryloxymethyl ketones as interleukin-1.beta. converting enzyme inhibitors
IN Dolle, Roland E.; Singh, Jasbir; Whipple, David A.; Prouty, Catherine; Chaturvedula, Prasad V.; Schmidt, Stanley J.; Awad, Mohamed M. A.; Hoyer, Denton W.; Ross, Tina M.
PA Sanofi Winthrop Inc., USA
SO U.S., 17 pp., Cont.-in-part of U.S. Ser. No. 237, 920, abandoned.
CODEN: USXXAM
DT **Patent**
LA English
IC ICM A61K038-00
ICS A61K031-415; C07K005-00; C07D231-04
NCL 514018000
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 63
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5585357	A	19961217	US 1996-593773	19960129 <--
	JP 07089951	A2	19950404	JP 1994-119873	19940601 <--
	CA 2125021	AA	19941204	CA 1994-2125021	19940602 <--
	AU 9463473	A1	19950427	AU 1994-63473	19940602 <--
	AU 690102	B2	19980423		
	IL 109867	A1	19980715	IL 1994-109867	19940602 <--
	FI 9402624	A	19941204	FI 1994-2624	19940603 <--
	NO 9402064	A	19941205	NO 1994-2064	19940603 <--
	HU 68689	A2	19950728	HU 1994-1679	19940603 <--
	HU 75964	A2	19970528	HU 1996-2985	19950428 <--
	US 5677283	A	19971014	US 1996-732173	19961016 <--
PRAI	US 1993-71623		19930603	<--	
	US 1994-237920		19940429	<--	
	US 1994-236425		19940429	<--	
	US 1996-593773		19960129	<--	

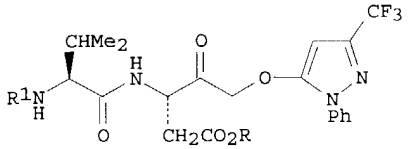
CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 5585357	ICM	A61K038-00
	ICS	A61K031-415; C07K005-00; C07D231-04
	NCL	514018000

OS MARPAT 126:144549
GI



I



II

AB Title compds. I [each AA = independently L-Val, L-Ala; N-methylalanine, N-methylvaline; R1 = 4-Me2NCH2C6H4CO, PhCH2O2C (Z), PhCH2CO, (4-pyridylmethyl)carbonyl, 3-piperidinopropionyl, 4-(morpholinoethoxy)benzoyl, 2-quinuclidinylcarbonyl, (3-pyridyl)methoxycarbonyl, (2-pyridyl)methoxycarbonyl, (4-phenylpiperazino)carbonyl; R8, R9, R10 = independently H, lower alkyl, halo-substituted Me, carbalkoxy, PhCH2, Ph, or Ph mono or disubstituted with F, NO2, MeO, Cl, CF3, MeSO2] which inhibit interleukin-1.beta. protease activity, pharmaceutical compns. containing the compds. and methods using the compds. are provided (no data). Thus, substitution of protected dipeptide bromomethyl ketone Z-L-Val-L-Asp(OCMe3)-CH2Br with 1-phenyl-3-trifluoromethyl-5-pyrazolone gave ester II (R = CMe3, R1 = Z) in 85% yield. Hydrogenolysis of the Z group, acylation with 4-(Me2NCH2)C6H4COCl, and acidic deesterification gave title compound II [R = H, R1 = 4-(Me2NCH2)C6H4CO] in 50% yield.

ST peptidyl heteroaryloxymethyl ketone prepn enzyme inhibitor; interleukin converting enzyme inhibitor heteroaryloxymethyl ketone

IT Ketones, preparation
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(peptidyl, heteroaryloxymethyl; preparation of peptidyl heteroaryloxymethyl ketones as interleukin-1.beta. converting enzyme inhibitors)

IT 9001-92-7, Protease
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(Interleukin-1.beta.; preparation of peptidyl heteroaryloxymethyl ketones as interleukin-1.beta. converting enzyme inhibitors)

IT 159391-12-5P 159391-13-6P 159391-14-7P 159391-18-1P 159391-21-6P
168318-05-6P 168318-06-7P 168318-07-8P 168318-08-9P 168318-10-3P
168318-12-5P 168318-13-6P 168318-14-7P 168318-15-8P 168318-16-9P
168318-17-0P 168318-18-1P 168318-19-2P 168318-20-5P 168318-21-6P
168318-22-7P 168318-23-8P 168318-24-9P 168318-26-1P 168318-27-2P
168318-28-3P 168318-29-4P 168318-30-7P 168318-32-9P 168318-34-1P
168318-35-2P 168318-36-3P 168318-37-4P 168318-39-6P 168318-40-9P
168318-43-2P 168318-45-4P 168318-46-5P 168318-47-6P 168318-48-7P
168318-49-8P 168318-51-2P 168318-52-3P 168318-53-4P 168318-54-5P
168318-55-6P 168318-56-7P 168318-57-8P 168318-60-3P 168318-61-4P
168318-62-5P 168318-63-6P 168318-64-7P 168318-65-8P 168318-66-9P
168318-67-0P 168318-68-1P 168318-69-2P 168318-72-7P 168318-73-8P
168318-74-9P 168318-75-0P 168318-76-1P 168318-77-2P 168318-78-3P
168318-79-4P 168318-80-7P 168318-82-9P 168318-85-2P 168318-86-3P
168318-87-4P 168318-88-5P 168318-89-6P 168318-93-2P 168318-94-3P
168608-14-8P 186498-51-1P 186498-52-2P 186498-53-3P 186498-54-4P
186498-55-5P 186498-56-6P 186498-57-7P 186498-58-8P 186498-59-9P
186498-60-2P 186498-61-3P 186498-62-4P 186498-63-5P 186498-64-6P
186498-65-7P **186498-66-8P** 186498-67-9P 186498-68-0P
186498-69-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); **SPN (Synthetic preparation)**; THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of peptidyl heteroaryloxymethyl ketones as interleukin-1.beta. converting enzyme inhibitors)

IT 321-07-3, 1-Phenyl-3-trifluoromethyl-5-pyrazolone 1076-38-6,

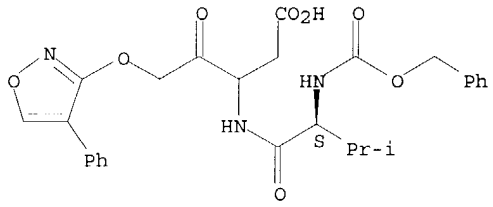
4-Hydroxycoumarin 1786-05-6, 4-Hydroxy-3-phenylcoumarin 16854-67-4, 4-Hydroxythiocoumarin 18469-52-8, Methyl 4-(aminomethyl)benzoate 21474-06-6, 4-Hydroxy-3-phenylisoxazole 23253-51-2, 5-Hydroxy-3-phenylisoxazole 27772-79-8 89819-63-6, 5-Hydroxy-3-(4-pyridinyl)isoxazole 134581-47-8 168319-04-8 168319-05-9 168319-06-0 186498-70-4 186498-72-6 186498-73-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of peptidyl heteroaryloxymethyl ketones as interleukin-1.beta. converting enzyme inhibitors)

IT 18364-71-1P 121811-18-5P, 4-(N,N-Dimethylaminomethyl)benzoyl chloride 168318-98-7P 168318-99-8P 168319-00-4P 168319-01-5P 168319-02-6P 186498-71-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of peptidyl heteroaryloxymethyl ketones as interleukin-1.beta. converting enzyme inhibitors)

IT **186498-66-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); **SPN (Synthetic preparation)**; THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation of peptidyl heteroaryloxymethyl ketones as interleukin-1.beta. converting enzyme inhibitors)

RN 186498-66-8 HCAPLUS
CN Pentanoic acid, 3-[[3-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]butyl]amino]-4-oxo-5-[(4-phenyl-3-isoxazolyl)oxy]-, [3(S)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L28 ANSWER 13 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:52859 HCAPLUS
DN 124:261059
ED Entered STN: 26 Jan 1996
TI Pyridazine derivatives useful as ligands of muscarinic cholinergic receptors
IN Boigegrain, Robert; Brodin, Roger; Kan, Jean P.; Olliero, Dominique; Bourguignon, Jean Jacques; Worms, Paul
PA Sanofi, Fr.
SO U.S., 28 pp. Cont.-in-part of U.S. Ser. No. 737, 654, abandoned.
CODEN: USXXAM
DT **Patent**
LA English
IC A61K031-50
NCL 514247000
CC 28-15 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63
FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5461053	A	19951024	US 1992-964901	19921022 <--
	FR 2642754	A1	19900810	FR 1989-1547	19890207 <--
	FR 2642754	B1	19910524		
	FR 2642757	A1	19900810	FR 1989-1548	19890207 <--
	FR 2642757	B1	19910524		
	FR 2654727	A1	19910524	FR 1989-15137	19891117 <--
	FR 2654727	B1	19920327		
	FR 2663326	A2	19911220	FR 1990-7533	19900615 <--
	FR 2663326	B2	19921016		
	FR 2665442	A1	19920207	FR 1990-9777	19900731 <--
	FR 2665442	B1	19921204		
	FI 9005663	A	19910518	FI 1990-5663	19901115 <--
	ZA 9009221	A	19910925	ZA 1990-9221	19901116 <--
	US 5631255	A	19970520	US 1995-473582	19950607 <--

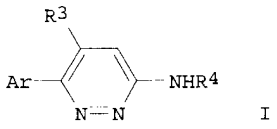
	US 5656631	A	19970812	US 1995-473580	19950607 <--
PRAI	FR 1989-1547		19890207	<--	
	FR 1989-1548		19890207	<--	
	FR 1989-15137		19891117	<--	
	US 1990-475489		19900207	<--	
	FR 1990-7533		19900615	<--	
	FR 1990-9777		19900731	<--	
	US 1990-615373		19901119	<--	
	US 1991-737654		19910730	<--	
	US 1992-871505		19920421	<--	
	US 1992-964901		19921022	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 5461053	IC	A61K031-50
	NCL	514247000

OS MARPAT 124:261059

GI



I

AB The present invention relates to pyridazine derivs. I in which: Ar represents a Ph group substituted by R1 and R2 ; R1 and R2 each independently denotes hydrogen, halogen, trifluoromethyl, hydroxyl, C1-C4 alkoxy or C1-C4 alkyl; R3 represents C3H7, C3-C7 cycloalkyl or the Ar' radical, Ar' being Ph substituted by R1 and R2 ; R4 represents the group CH2C(CH2X1)2(CH2)nNR5R6 in which: X1 represents hydrogen or methyl; n is 0; R5 represents a C1-C6 linear alkyl group; and R6 represents a C1-C6 linear alkyl group; or a group Alk-NR5aR6a in which Alk is a C1-C6 linear alkylene group, R5a is hydrogen or a C1-C6 alkyl group and R6a alkyl group, a benzyl or a C3-C7 cycloalkyl, with the proviso that R1 and R2 are not simultaneously H when Alk is (CH2)2, and that R4 is the group AlkNR5aR6a only when R3 is a C3H7 or a Ph group; or its salts, which are pharmaceutically acceptable or permit suitable separation or crystallization thereof, which are useful as ligands of cholinergic receptors, in particular, receptors of the M1 type. Thus, e.g., amination of 6-chloro-3-phenyl-4-propylpyridazine (preparation given) with 2-(dimethylamino)-2-methylpropylamine (preparation given) afforded a base which was converted to 3-(2-diethylamino-2-methylpropyl)amino-6-phenyl-5-propyl-pyridazine sesquifumarate (SR 46559A); SR 46559A exhibited IC50's of 0.11 and 2.2 .mu.mol, resp., representing affinity for M1 and M2 muscarinic cholinergic receptors. Pharmaceutical formulations were given.

ST pyridazine deriv ligand muscarinic cholinergic receptor

IT Nervous system
(central, cholinergic, disease, deficiency, treatment; pyridazine derivs. useful as ligands of muscarinic cholinergic receptors)

IT Receptors
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)
(muscarinic M1, pyridazine derivs. useful as ligands of muscarinic cholinergic receptors)

IT 132449-99-1P, SR 96185 132450-00-1P 132450-01-2P, SR 96194A
132450-02-3P, SR 96181 132450-03-4P, SR 96198 132450-04-5P, SR 96222
132450-05-6P, SR 46004A 132450-06-7P, SR 96204A 132450-07-8P, SR 96240A 132450-08-9P, SR 46005A 132450-09-0P, SR 45991A 132450-10-3P, SR 96220A 132450-11-4P, SR 96205A 132450-12-5P, SR 96239A
132450-13-6P, SR 46035A 132450-15-8P, SR 46079A 132450-16-9P, SR 96193A 132450-17-0P, SR 96197A 132450-18-1P, SR 96223A 132450-19-2P, SR 45964A 132450-20-5P, SR 45944A 132450-21-6P, SR 46179A
132450-23-8P, SR 46197A 132450-24-9P, SR 46222A 132450-27-2P, SR 46224A 132450-28-3P, SR 46405A 132450-30-7P, SR 46534A 132450-31-8P, SR 46431A 132450-32-9P, SR 46432A 132450-33-0P, SR 46514
132450-34-1P, SR 46637A 132450-35-2P, SR 46636A 132450-37-4P, SR 96224A 132450-39-6P, SR 96230A 132450-41-0P, SR 96266A 132450-42-1P, SR 96232A 132450-43-2P, SR 46010A 132450-44-3P, SR 46081A
132450-45-4P, SR 45960A 132450-46-5P, SR 46080A 132450-48-7P, SR 46731A 132450-50-1P, SR 96231A 132450-51-2P, SR 45961A 132450-52-3P, SR 45988A 132450-53-4P, SR 45989A 132450-54-5P, SR 46377A

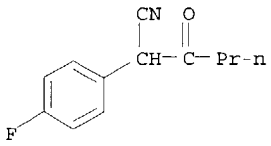
132450-56-7P, SR 46532A 132450-57-8P, SR 46728A 132450-59-0P, SR 96290A 132450-60-3P, SR 96291 132450-62-5P, SR 46352A 132450-64-7P, SR 46359A 132450-66-9P, SR 46378A 132450-68-1P, SR 46533A
132450-69-2P, SR 46180 132450-71-6P, SR 46195 132450-72-7P, SR 46196
132450-74-9P, SR 96269 132450-75-0P, SR 96272 132450-76-1P, SR 46433
132450-77-2P, SR 46434 132450-78-3P, SR 46430 132450-80-7P, SR 47046
132450-82-9P, SR 47186 132450-84-1P, SR 47226 132450-85-2P, SR 96305
132450-87-4P, SR 96307A 132450-88-5P, SR 96308A 132450-90-9P, SR 46457A 132450-92-1P, SR 46578A 132450-94-3P, SR 46640A 132471-76-2P, SR 46082A 132471-78-4P, SR 46730A 132471-79-5P, SR 96306A
136549-27-4P, SR 46729A 136549-29-6P, SR 46733A 136549-30-9P, SR 47675A 136549-31-0P, SR 47802A 136549-32-1P, SR 47803A 136549-33-2P, SR 47804A 136549-35-4P 136549-36-5P, SR 47047A 136549-37-6P, SR 47068 136549-38-7P, SR 47069A 136549-40-1P, SR 47227A 136549-41-2P, SR 47297A 136549-42-3P, SR 47608A 136549-43-4P, SR 47609A
136549-45-6P, SR 47890A 136549-46-7P, SR 47967 136549-47-8P, SR 48080
136549-48-9P, SR 48081A 136549-49-0P, SR 48082 136549-50-3P, SR 47674A
136577-30-5P, SR 47673 137733-33-6P, SR 46559A 137733-34-7P
137733-35-8P, SR 47883A 137733-37-0P, SR 47020A 137733-39-2P, SR 47054A 137733-41-6P, SR 47097A 137733-45-0P, SR 47138A 137733-49-4P, SR 47655A 137733-51-8P, SR 47878A 137733-53-0P, SR 48079A
137754-67-7P, SR 46732A 141234-76-6P 141234-78-8P 141234-79-9P
141234-80-2P 141234-81-3P 141234-83-5P 141234-88-0P 141234-90-4P
141234-92-6P 141234-94-8P 141234-96-0P 141234-98-2P 141235-00-9P
141235-04-3P 141235-05-4P 141235-06-5P 141235-07-6P 141235-09-8P
141235-10-1P 141235-11-2P 141235-13-4P 149453-82-7P, SR 96376
174700-29-9P 174700-32-4P 174700-33-5P 174700-34-6P 174700-35-7P
174756-84-4P, SR 47098A 174794-12-8P, SR 47153A 174794-13-9P, SR 96268
174794-14-0P, SR 46641A
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(pyridazine derivs. useful as ligands of muscarinic cholinergic receptors)

IT 75-86-5, Acetone cyanohydrin 93-55-0, Propiophenone 100-36-7, N,N-Diethylethylenediamine 105-54-4, Ethyl butyrate 109-89-7, reactions 115-11-7, reactions 121-97-1 459-22-3, (4-Fluorophenyl)acetonitrile 924-44-7, Ethyl glyoxylate 1009-14-9, Valerophenone 26116-12-1, 2-(Aminomethyl)-1-ethylpyrrolidine
132451-09-3, 3-Chloro-6-(2-methoxyphenyl)-5-methylpyridazine
RL: RCT (Reactant); RACT (Reactant or reagent)
(pyridazine derivs. useful as ligands of muscarinic cholinergic receptors)

IT 3378-38-9P 21404-84-2P, 2-Diethylamino-2-methylpropionamide
21404-89-7P, 2-Diethylamino-2-methylpropylamine 27062-58-4P
33048-55-4P, 5-Methyl-6-phenyl-2H-pyridazin-3-one 35672-46-9P, 2-Diethylamino-2-methylpropionitrile 66549-28-8P 67820-83-1P
68415-28-1P 70777-03-6P 108302-59-6P 127867-89-4P, 5-Methyl-6-(4-methoxyphenyl)-2H-pyridazin-3-one 132450-98-7P
132450-99-8P 132451-00-4P 132451-01-5P 132451-02-6P 132451-03-7P
132451-04-8P 132451-05-9P 132451-06-0P 132451-07-1P 132451-08-2P
132451-10-6P 132451-11-7P 132451-12-8P 136549-25-2P 136549-34-3P, 6-Phenyl-5-propyl-2H-pyridazin-3-one 136549-51-4P 136549-52-5P
136549-53-6P 136549-54-7P 136549-55-8P 136549-56-9P 136549-57-0P
136549-58-1P 136549-59-2P 136549-60-5P 136549-61-6P 136549-62-7P
136549-63-8P 136549-64-9P 136549-65-0P 136549-66-1P 141235-14-5P, 1-(4-Fluorophenyl)pentan-2-one 141235-16-7P 141235-18-9P
141235-19-0P 141235-20-3P 141235-21-4P 141235-22-5P 141235-23-6P
141235-24-7P 141235-25-8P 141235-26-9P 141235-27-0P 141235-28-1P
141235-29-2P 141235-30-5P 141235-31-6P 141235-32-7P 141235-33-8P
141235-34-9P 141235-35-0P 141235-36-1P 141235-37-2P 141235-38-3P
141235-39-4P 141235-40-7P 141235-41-8P 141235-42-9P 141235-43-0P
141235-44-1P 141235-45-2P 141235-46-3P 141235-47-4P 141235-48-5P
141235-49-6P 141235-50-9P 141235-51-0P 174700-28-8P 174700-30-2P
174700-36-8P, .alpha.-Butyryl-(4-fluorophenyl)acetonitrile
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(pyridazine derivs. useful as ligands of muscarinic cholinergic receptors)

IT **174700-36-8P**, .alpha.-Butyryl-(4-fluorophenyl)acetonitrile
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(pyridazine derivs. useful as ligands of muscarinic cholinergic receptors)

RN 174700-36-8 HCAPLUS
CN Benzeneacetonitrile, 4-fluoro-.alpha.-(1-oxobutyl)- (9CI) (CA INDEX NAME)



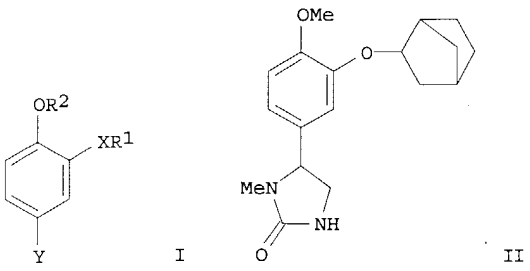
L28 ANSWER 14 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:931617 HCAPLUS
DN 124:146130
ED Entered STN: 21 Nov 1995
TI [Alkoxy[(polycycloalkyl)oxy- and -amino]phenyl]heterocyclic calcium independent c-AMP phosphodiesterase inhibitor antidepressants
IN Saccomano, Nicholas A.; Vinick, Fredric J.
PA Pfizer Inc., USA
SO U.S., 29 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC ICM C07D239-36
ICS A61K031-505
NCL 514274000
CC 28-1 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 27, 63
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	US 5459145	A	19951017	US 1988-155932	19880119	<--
	US 5128358	A	19920707	US 1991-696690	19910530	<--
	US 5196426	A	19930323	US 1992-854136	19920319	<--
	US 5294730	A	19940315	US 1992-984190	19921120	<--
	US 5414127	A	19950509	US 1994-184092	19940119	<--
PRAI	US 1988-155932	A3	19880119	<--		
	US 1991-696690	A3	19910830	<--		
	US 1992-854136	A3	19920319	<--		
	US 1992-984190	A3	19921120	<--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 5459145	ICM	C07D239-36
	ICS	A61K031-505
	NCL	514274000
US 5459145	ECLA	C07C217/60; C07C255/37; C07D233/32; C07D233/42; C07D233/78; C07D239/10B; C07D239/22D1; C07D029/36B; C07D285/08B; C07D285/10B; C07D487/04; C07D487/04 <--

OS MARPAT 124:146130
GI



AB Title compds. I wherein R1 is selected from the group consisting of bicyclo[2.2.1]heptyl, bicyclo[2.2.2]octyl, bicyclo[3.2.1]octyl, tricyclo[5.2.1.02,6]decyl, tricyclo[3.3.1.13,7]decyl and indanyl; R2 is Me or Et, X is O or NH; and Y comprises a 5- or 6-membered heterocyclic ring having one or two nitrogens; or fused bicyclic heterocyclic rings having a total of three nitrogen atoms, one in each ring and one angular nitrogen

(no data for antidepressant activity) are prepared as antidepressant agents (no data). Thus, e.g., treatment of 3-(bicyclo[2.2.1]hept-2-yloxy)-4-methoxybenzaldehyde (7:3 endo:exo mixture, preparation given) with NaCN/methylamine hydrochloride afforded a 7:3 endo:exo mixture of cyanoamines; the latter were reduced to 2-methylamino-2-[3-(bicyclo[2.2.1]hept-2-yloxy)-4-methoxyphenyl]ethylamine as a 7:3 endo to exo mixture and cyclized to 1-methyl-5-[3-(bicyclo[2.2.1]hept-2-yloxy)-4-methoxyphenyl]-2-imidazolidinone (II; 17.8%).

ST polycycloalkyloxyphenylheterocyclic calcium independent cAMP phosphodiesterase inhibitor; antidepressant polycycloalkyloxyphenylheterocycle; heterocycle polycycloalkyloxyphenyl antidepressant; polycycloalkylaminophenylheterocyclic calcium independent cAMP phosphodiesterase inhibitor

IT Antidepressants
([alkoxy[(polycycloalkyl)oxy- and -amino]phenyl]heterocyclic calcium independent c-AMP phosphodiesterase inhibitor antidepressants)

IT 115897-70-6P 115897-84-2P 115897-98-8P 115898-36-7P 144034-03-7P 144034-05-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
([alkoxy[(polycycloalkyl)oxy- and -amino]phenyl]heterocyclic calcium independent c-AMP phosphodiesterase inhibitor antidepressants)

IT 115897-71-7P 115897-73-9P 115897-74-0P 115897-75-1P 115897-76-2P
115897-77-3P 115897-80-8P 115897-83-1P 115897-87-5P 115897-90-0P
115897-93-3P 115897-96-6P 115897-97-7P 115898-00-5P 115898-05-0P
115898-06-1P 115898-07-2P 115898-08-3P 115898-19-6P 115898-23-2P
115898-24-3P 115898-25-4P 115898-26-5P 115898-29-8P 115898-30-1P
115898-34-5P 115919-88-5P 144033-88-5P 144033-96-5P 144033-97-6P
144033-98-7P 144033-99-8P 144034-00-4P 144034-06-0P 144034-07-1P
173252-99-8P 173253-00-4P 173253-01-5P 173253-02-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
([alkoxy[(polycycloalkyl)oxy- and -amino]phenyl]heterocyclic calcium independent c-AMP phosphodiesterase inhibitor antidepressants)

IT 9036-21-9, c-AMP phosphodiesterase
RL: BSU (Biological study, unclassified); BIOL (Biological study)
([alkoxy[(polycycloalkyl)oxy- and -amino]phenyl]heterocyclic calcium independent c-AMP phosphodiesterase inhibitor antidepressants)

IT 64-04-0, Phenethylamine 105-53-3, Diethyl malonate 120-80-9, Pyrocatechol, reactions 372-09-8, Cyanoacetic acid 497-36-9, Endo-Bicyclo[2.2.1]heptan-2-ol 497-38-1, Norcamphor 542-69-8, 1-Iodobutane 621-59-0, Isovanillin 700-57-2, 2-Adamantanol 931-64-6, Bicyclo[2.2.2]-2-octene 1702-10-9 1820-80-0, 3-Aminopyrazole 2534-77-2, exo-2-Bromonorbornane 5762-56-1, Tris(dimethylamino)methane 6351-10-6, 1-Indanol 7374-90-5 13380-89-7, Tricyclo[5.2.1.02,6]decan-8-ol 13380-94-4, Tricyclo[5.2.1.02,6]decan-8-one 29804-62-4, Bicyclo[3.2.1]octan-3-ol 31680-08-7, 4-Methoxy-3-nitrobenzaldehyde 42383-61-9, 2-Aminoimidazole sulfate 50447-20-6 94277-20-0 113034-45-0 115898-77-6
RL: RCT (Reactant); RACT (Reactant or reagent)
([alkoxy[(polycycloalkyl)oxy- and -amino]phenyl]heterocyclic calcium independent c-AMP phosphodiesterase inhibitor antidepressants)

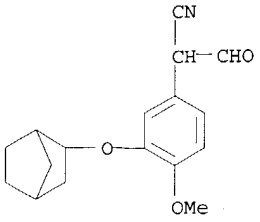
IT 18684-63-4P, Bicyclo[2.2.2]octan-2-ol 56137-56-5P 115897-62-6P
115897-63-7P 115897-65-9P 115897-66-0P 115897-67-1P 115897-69-3P
115897-78-4P 115897-79-5P 115897-81-9P 115897-82-0P 115897-85-3P
115897-86-4P 115897-88-6P 115897-89-7P 115897-91-1P 115897-92-2P
115897-94-4P 115897-95-5P 115897-99-9P **115898-01-6P**
115898-02-7P 115898-03-8P 115898-04-9P 115898-09-4P
115898-10-7P 115898-11-8P 115898-12-9P 115898-16-3P 115898-17-4P
115898-18-5P 115898-20-9P 115898-21-0P 115898-22-1P 115898-38-9P
115898-39-0P 115898-42-5P 115898-47-0P 115898-48-1P 115898-49-2P
115898-50-5P 115898-51-6P 115898-52-7P 115898-53-8P 115898-54-9P
115898-55-0P 115898-56-1P 115898-57-2P 115898-58-3P 115898-59-4P
115898-62-9P 115898-63-0P 115898-64-1P 115898-65-2P 115898-66-3P
115898-67-4P 115898-68-5P 115898-69-6P 115898-70-9P 115898-71-0P
115898-72-1P 115898-73-2P 115898-74-3P 115898-75-4P 115898-76-5P
115898-78-7P 115919-89-6P 131408-38-3P 131408-40-7P 131486-67-4P
131486-68-5P 144033-87-4P 144033-93-2P 144034-04-8P 144034-16-2P
144034-17-3P 144124-74-3P 173252-95-4P 173252-96-5P 173252-97-6P
173252-98-7P 173327-35-0P 173327-36-1P
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
([alkoxy[(polycycloalkyl)oxy- and -amino]phenyl]heterocyclic calcium

independent c-AMP phosphodiesterase inhibitor antidepressants)

IT **115898-01-6P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
([alkoxy[(polycycloalkyl)oxy- and -amino]phenyl]heterocyclic calcium independent c-AMP phosphodiesterase inhibitor antidepressants)

RN 115898-01-6 HCAPLUS

CN Benzeneacetonitrile, 3-(bicyclo[2.2.1]hept-2-yloxy)-.alpha.-formyl-4-methoxy- (9CI) (CA INDEX NAME)



L28 ANSWER 15 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1995:708473 HCAPLUS

DN 123:83209

ED Entered STN: 29 Jul 1995

TI Anti-estrogenic compounds and compositions

IN Labrie, Fernand; Merand, Yves

PA Endorecherche Inc., Can.

SO U.S., 72 pp. Cont.-in-part of U.S. Ser. No. 265,150, abandoned.
CODEN: USXXAM

DT **Patent**

LA English

IC ICM A61K031-445
ICS A61K031-44; A61K031-545; C07D401-00

NCL 514320000

CC 27-14 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 2, 32

FAN.CNT 8

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 5395842	A	19950307	US 1991-801704	19911202 <--
HU 52114	A2	19900628	HU 1989-5469	19891027 <--
HU 208150	B	19930830		
JP 2000256390	A2	20000919	JP 2000-62592	19891031 <--
US 5393785	A	19950228	US 1992-913746	19920714 <--
WO 9310741	A2	19930610	WO 1992-CA518	19921201 <--
WO 9310741	A3	19940203		
W: AU, BB, BG, BR, CA, CS, FI, HU, JP, KP, KR, LK, MG, MN, MW, NO, NZ, PL, PT, RO, RU, SD				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
AU 9229393	A1	19930628	AU 1992-29393	19921201 <--
AU 681338	B2	19970828		
ZA 9209309	A	19940601	ZA 1992-9309	19921201 <--
EP 615448	A1	19940921	EP 1992-923641	19921201 <--
EP 615448	B1	20020502		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, SE				
RU 2142945	C1	19991220	RU 1994-31127	19921201 <--
IL 103941	A1	20000726	IL 1992-103941	19921201 <--
JP 2002060384	A2	20020226	JP 2001-207820	19921201 <--
AT 216880	E	20020515	AT 1992-923641	19921201 <--
ES 2176190	T3	20021201	ES 1992-923641	19921201 <--
US 5631249	A	19970520	US 1993-17045	19930212 <--
NO 9402027	A	19940704	NO 1994-2027	19940601 <--
FI 9402568	A	19940727	FI 1994-2568	19940601 <--
US 5840735	A	19981124	US 1994-285354	19940803 <--
US 6060503	A	20000509	US 1995-388207	19950221 <--
US 5686437	A	19971111	US 1995-475710	19950607 <--
US 5686465	A	19971111	US 1995-485739	19950607 <--
AU 9746772	A1	19980219	AU 1997-46772	19971128 <--
JP 10273479	A2	19981013	JP 1998-10654	19980122 <--
JP 3273010	B2	20020408		
AU 760232	B2	20030508	AU 2000-20637	20000303 <--

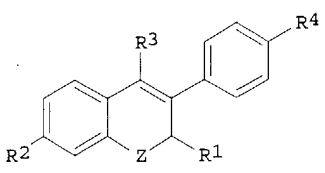
	AU 762751	B2	20030703	AU 2000-34056	20000512 <--
	AU 2000034056	A5	20000720		
PRAI	US 1988-265150	B2	19881031	<--	
	US 1989-377010	B2	19890707	<--	
	US 1988-265716	A	19881101	<--	
	US 1989-322154	A	19890310	<--	
	JP 1989-286010	A3	19891031	<--	
	US 1991-801704	A	19911202	<--	
	US 1992-917915	A3	19920719	<--	
	JP 1993-509666	A3	19921201	<--	
	JP 1998-10654	A3	19921201	<--	
	WO 1992-CA518	A	19921201	<--	
	US 1993-17045	A3	19930212	<--	
	US 1994-285354	A2	19940803	<--	
	AU 1996-46606	A3	19960220	<--	
	AU 1997-46772	A3	19971128	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 5395842	ICM	A61K031-445
	ICS	A61K031-44; A61K031-545; C07D401-00
	NCL	514320000
US 5395842	ECLA	A61K031/10; A61K031/135; A61K031/165; A61K031/35; A61K031/38; A61K031/40; A61K031/445; A61K031/47; C07C217/18; C07C235/34; C07C317/18; C07D215/14; C07D217/16; C07D235/18; C07D295/0A3; C07D295/08B1D8B; C07D295/18B1D; C07D311/60; C07D335/06A; C07J001/00B2; C07J001/00B4B; C07J001/0B4B1; C07J001/00C5B; C07J001/00C5; C07J001/00C1; C07J001/00C2; C07J001/00C4B; C07J001/00C4B1; C07J001/00CC2; C07J017/00; C07J021/00C1; C07J021/00C2; C07J041/00C40; C07J041/00C70; C07J051/00; C07J053/00C1D; C07J071/00B1; C07J071/00B1C <--
US 5631249	ECLA	A61K031/10; A61K031/135; A61K031/138; A61K031/165; A61K031/352; A61K031/382; A61K031/40; A61K031/40P5; A61K031/4535; A61K031/47; A61K031/47J; A61K031/4709; A61K031/4725; A61K031/575; A61K031/58; A61K031/585; C07C235/34; C07D235/18; C07J001/00B5C2; C07J001/00B5C1; C07J001/00B4B1; C07J001/00B4B; C07J001/00B2; C07J001/00C5C2; C07J001/00C5; C07J001/00C4B1; C07J001/00C4B; C07J001/00C2; C07J001/00C1; C07J017/00; C07J021/00C2; C07J021/00C1; C07J041/00C3; C07J041/00C4D; C07J041/00C40; C07J041/00C60; C07J041/00C70; C07J051/00; C07J053/00C1D; C07J071/00B1; A61K031/4025; A61K031/453 <--
US 5686437	ECLA	A61K031/10; C07J041/00C40; C07J041/00C60; C07J041/00C70; C07J051/00; C07J053/00C1D; C07J071/00B1C; C07J071/00B1; A61K031/135; A61K031/138; A61K031/165; A61K031/352; A61K031/382; A61K031/40; A61K031/40P5; A61K031/4025; A61K031/453; A61K031/4535; A61K031/47; A61K031/47J; A61K031/4709; A61K031/4725; A61K031/575; A61K031/58; A61K031/585; C07C235/34; C07D235/18; C07J001/00B5C2; C07J001/00B5C1; C07J001/00B2; C07J001/00B4B; C07J001/00B4B1; C07J001/00C5; C07J001/00C1; C07J001/00C2; C07J001/00C4B; C07J001/00C4B1; C07J001/00C5C2; C07J017/00; C07J021/00C1; C07J021/00C2; C07J041/00C3; C07J041/00C4D <--

OS MARPAT 123:83209

GI



I

AB Title compds. I [Z = alkylene, haloalkylene, oxaalkylene, thiaalkylene, azaalkylene; R1 = substituted phenylene; R2, R4 = H, OH, protected OH; R3 = H, aliphatic] and their 3,4-dihydro derivs. and pharmaceutical compns. containing them were prepared Such pharmaceutical compns. are useful for the

treatment of breast cancer or other diseases whose progress is aided by activation of sex steroid receptors. Thus, I [Z = O, R1 = 4-(2-piperidinoethoxy)phenyl, R2, R4 = OH, R3 = Me, II] was prepared from 2,4-(MeO)2C6H3COCl in 9 steps. II had an ED50 for inhibition of ZR-75-1 cells of 2.55X10-10 M.

ST diarylbenzopyranol prepn antiestrogenic; neoplasm inhibitor diarylbenzopyranol; benzopyranol diaryl prepn antiestrogenic

IT Neoplasm inhibitors
(preparation of antiestrogenic diarylbenzopyrans and related compds.)

IT Estrogens
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(antiestrogens, preparation of antiestrogenic diarylbenzopyrans and related compds.)

IT 131811-94-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(9repn. of antiestrogenic diarylbenzopyrans and related compds.)

IT 131811-54-6P 134227-19-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of antiestrogenic diarylbenzopyrans and related compds.)

IT 104-47-2, 4-Methoxyphenylacetonitrile 123-08-0 434-22-0, 19-Nortestosterone 1440-60-4, N-Chloroacetylpiperidine 1611-56-9, 11-Bromo-1-undecanol 2008-75-5, 1-(2-Chloroethyl)piperidine hydrochloride 2398-37-0, 3-Bromoanisole 2472-22-2 3143-02-0 3589-92-2 3647-69-6, 4-(2-Chloroethyl)morpholine hydrochloride 4390-94-7 39096-59-8 39828-35-8, 2,4-Dimethoxybenzoyl chloride 52056-69-6 103483-33-6 151533-59-4 151533-66-3 151533-68-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of antiestrogenic diarylbenzopyrans and related compds.)

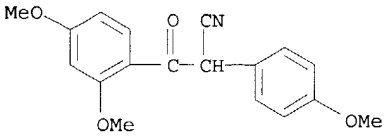
IT 2150-41-6P, Methyl 2,4-dimethoxybenzoate 2590-41-2P 4999-76-2P 17720-60-4P 39604-64-3P 55592-08-0P 55592-09-1P 55592-10-4P 55592-11-5P 67804-60-8P 98008-56-1P 98013-89-9P 127947-01-7P 127947-02-8P 130064-21-0P 130064-26-5P 130064-27-6P 131811-57-9P 131811-59-1P 131811-61-5P 131811-71-7P 131811-72-8P 131811-73-9P 131811-74-0P 131811-75-1P 131811-76-2P 131811-77-3P 131811-78-4P 131811-79-5P 131811-80-8P 131811-81-9P 131811-82-0P 131811-83-1P 131811-84-2P 131811-85-3P 131811-86-4P 131811-87-5P 131811-88-6P 131811-89-7P 131811-90-0P 131811-91-1P 131811-92-2P 131811-93-3P 131811-95-5P 131811-96-6P 131838-68-1P **132593-12-5P** 151533-32-3P 151533-33-4P 151533-35-6P 151533-39-0P 151533-44-7P 151533-45-8P 151533-46-9P 151533-52-7P 151533-55-0P 151533-57-2P 151533-61-8P 151533-64-1P 151533-67-4P 165535-11-5P 165535-12-6P 165535-13-7P 165535-14-8P
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of antiestrogenic diarylbenzopyrans and related compds.)

IT 131811-52-4P 131811-53-5P 131811-55-7P 131811-56-8P 131811-58-0P 131811-60-4P 131811-64-8P 131811-65-9P 131811-66-0P 131811-70-6P 151533-34-5P 151533-50-5P 151533-53-8P 151533-56-1P 151533-58-3P 151533-62-9P 151533-65-2P 151533-72-1P 151533-76-5P 151533-77-6P 165535-15-9P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of antiestrogenic diarylbenzopyrans and related compds.)

IT **132593-12-5P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation of antiestrogenic diarylbenzopyrans and related compds.)

RN 132593-12-5 HCAPLUS

CN Benzenepropanenitrile, 2,4-dimethoxy-.alpha.-(4-methoxyphenyl)-.beta.-oxo- (9CI) (CA INDEX NAME)



L28 ANSWER 16 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

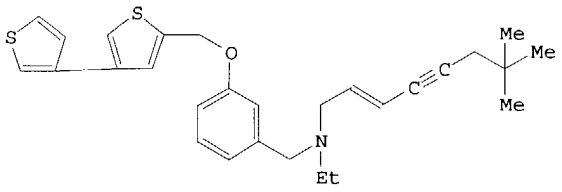
AN 1994:435005 HCAPLUS
DN 121:35005
ED Entered STN: 23 Jul 1994
TI Substituted alkylamine derivatives
IN Takezawa, Hiroshi; Hayashi, Masahiro; Iwasawa, Yoshikazu; Hosoi, Masaaki; Iida, Yoshiaki; Tsuchiya, Yoshimi; Horie, Masahiro; Kamei, Toshio
PA Banyu Pharmaceutical Co., Ltd., Japan
SO U.S., 74 pp. Cont.-in-part of U.S. Ser. No. 533,532, abandoned.
CODEN: USXXAM
DT **Patent**
LA English
IC ICM A61K031-38
ICS C07D333-32
NCL 514444000
CC 25-5 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1, 27, 28
FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5234946	A	19930810	US 1991-753611	19910830 <--
	ZA 8808792	A	19890830	ZA 1988-8792	19881124 <--
	JP 03193746	A2	19910823	JP 1988-296840	19881124 <--
	CN 1037141	A	19891115	CN 1988-109274	19881126 <--
	ZA 8908464	A	19910130	ZA 1989-8464	19891107 <--
PRAI	JP 1987-299584		19871127	<--	
	JP 1988-96286		19880419	<--	
	JP 1988-113310		19880510	<--	
	JP 1988-285381		19881111	<--	
	US 1988-274972		19881122	<--	
	US 1990-465209		19900308	<--	
	US 1990-533532		19900605	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 5234946	ICM	A61K031-38
	ICS	C07D333-32
	NCL	514444000

OS MARPAT 121:35005
GI



I

AB The title compds. and their uses for the treatment of hypercholesteremia, arteriosclerosis and and hyperlipemia are claimed. Specifically claimed is compound I. The title compds. are squalane epoxidase inhibitors.
ST fungicide benzylamine alkenynyl prepn; anticholesteremic benzylamine alkenynyl prepn; hyperlipemia benzylamine alkenynyl prepn; antiarteriosclerotic benzylamine alkenynyl prepn; squalane epoxidase inhibitor benzylamine alkenynyl prepn
IT Antiarteriosclerotics
Anticholesteremics and Hypolipemics
Fungicides and Fungistats
((alkenynyl)benzylamines and analogs)
IT 123924-95-8P 123925-11-1P 123925-36-0P 123925-55-3P 123926-00-1P
155293-40-6P 155293-41-7P 155293-42-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as antiarteriosclerotic, anticholesteremic or fungicide)
IT 123925-66-6P 123925-67-7P 123925-68-8P 123925-69-9P 123925-70-2P
123925-71-3P 123925-72-4P 123926-06-7P 123926-07-8P 123926-08-9P
123926-09-0P 123926-10-3P 123926-11-4P 123926-12-5P 123926-13-6P
123926-14-7P 123926-15-8P 123926-16-9P 123926-17-0P 123926-18-1P
123926-19-2P 123926-21-6P 123926-22-7P 123944-72-9P 129746-48-1P
129777-49-7P 131060-14-5P 134865-51-3P 136719-25-0P 136719-27-2P
136719-28-3P 136719-29-4P 136719-30-7P 136719-32-9P 155293-39-3P

155293-43-9P 155293-44-0P 155293-45-1P 155293-46-2P 155293-47-3P
155293-48-4P 155293-49-5P 155293-50-8P 155293-51-9P 155293-52-0P
155293-53-1P 155293-54-2P 155293-55-3P 155293-56-4P
155293-57-5P 155293-58-6P 155293-59-7P 155293-60-0P 155293-61-1P
155293-62-2P 155293-63-3P 155293-64-4P 155293-65-5P 155293-66-6P
155293-67-7P 155293-68-8P 155293-69-9P 155293-70-2P 155293-71-3P
155293-72-4P 155293-73-5P 155293-74-6P 155293-75-7P 155293-76-8P
155293-77-9P 155293-78-0P 155293-79-1P 155293-80-4P 155293-81-5P
155293-82-6P 155293-83-7P 155293-84-8P 155293-85-9P 155293-86-0P
155293-87-1P 155293-88-2P 155293-89-3P 155293-90-6P 155293-91-7P
155293-92-8P 155293-93-9P 155293-94-0P 155293-95-1P 155293-96-2P
155293-97-3P 155293-98-4P 155293-99-5P 155294-00-1P 155294-01-2P
155294-02-3P 155294-03-4P 155294-04-5P 155294-05-6P 155294-06-7P
155294-07-8P 155294-08-9P 155294-09-0P 155294-10-3P 155294-11-4P
155294-12-5P 155294-13-6P 155294-14-7P 155294-15-8P 155294-16-9P
155294-17-0P 155294-18-1P 155294-19-2P 155294-20-5P 155294-21-6P
155294-22-7P 155294-23-8P 155294-24-9P 155294-25-0P 155294-26-1P
155294-27-2P 155294-28-3P 155294-29-4P 155294-30-7P 155294-31-8P
155294-32-9P 155294-33-0P 155294-34-1P 155294-35-2P 155294-36-3P
155294-37-4P 155294-38-5P 155294-39-6P 155294-40-9P 155294-41-0P
155294-42-1P 155294-43-2P 155294-44-3P 155294-45-4P 155294-46-5P
155294-47-6P 155294-48-7P 155294-49-8P 155294-50-1P 155294-51-2P
155294-52-3P 155294-53-4P 155294-54-5P 155294-55-6P 155294-56-7P
155294-57-8P 155294-58-9P 155294-59-0P 155294-60-3P 155294-61-4P
155294-62-5P
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of, as antiarteriosclerotic, anticholesteremic or hypolipemic)

IT 78629-21-7P 123926-61-4P 129746-42-5P, 3-(3-Thienyl)benzaldehyde
129746-44-7P 129747-36-0P 129747-37-1P 129747-72-4P 136719-34-1P
155294-74-9P 155294-75-0P 155294-76-1P 155294-77-2P 155294-78-3P
155294-79-4P 155294-80-7P 155294-81-8P 155294-82-9P,
[2,3'-Bithiophene]-4-methanol 155294-83-0P 155294-84-1P 155294-85-2P
155294-86-3P 155294-87-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for (alkenynyl)benzylamine
(anticholesteremic, antiarteriosclerotic))

IT 155294-72-7P 155294-73-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for (alkenynyl)furfurylamine
(anticholesteremic, antiarteriosclerotic))

IT 155294-92-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for (alkenynyl)oxazolemethanamine
(anticholesteremic, antiarteriosclerotic))

IT 155294-89-6P 155294-90-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for (alkenynyl)thiophenemethanamine
(anticholesteremic, antiarteriosclerotic))

IT 1008-74-8, 5-(3-Methylphenyl)isoxazole 4515-89-3, 1-
Methylcyclopropanecarboxaldehyde 6138-90-5, Geranyl bromide
24033-03-2, 3-Benzyloxybenzyl chloride 39687-95-1, Methyl
isocyanoacetate 67978-51-2 67978-52-3 76100-81-7 89929-93-1,
3-(2-Furyl)benzyl alcohol 116939-14-1 123925-85-9 123926-30-7
123926-39-6 123926-40-9 123926-41-0 123926-54-5 123926-55-6
123926-61-4 129746-41-4 129747-33-7 129747-34-8 129747-39-3
129747-59-7 136719-31-8 136719-33-0, [3,3'-Bithiophene]-5-methanol
138139-92-1 155294-63-6 155294-64-7 155294-65-8 155294-66-9
155294-67-0 155294-68-1 155294-69-2 155294-70-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for (alkenynyl)benzylamine (anticholesteremic,
antiarteriosclerotic))

IT 89929-85-1, 3-(3-Thienyl)benzyl bromide 129777-47-5 155294-71-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for (alkenynyl)furfurylamine (anticholesteremic,
antiarteriosclerotic))

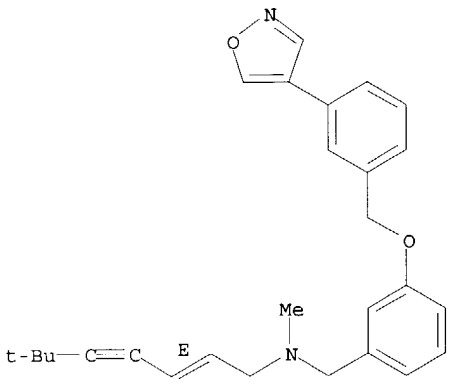
IT 155294-93-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for (alkenynyl)isoxazolemethanamine (anticholesteremic,
antiarteriosclerotic))

IT 155294-91-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for (alkenynyl)oxazolemethanamine (anticholesteremic,
antiarteriosclerotic))

IT 155294-88-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant for (alkenynyl)thiophenemethanamine (anticholesteremic,

antiarteriosclerotic))
IT 132052-93-8, Epoxidase
RL: RCT (Reactant); RACT (Reactant or reagent)
(squalane epoxidase inhibitors, (alkenynyl)benzylamines and analogs)
IT **155293-53-1P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of, as antiarteriosclerotic, anticholesteremic or hypolipemic)
RN 155293-53-1 HCAPLUS
CN Benzenemethanamine, N-(6,6-dimethyl-2-hepten-4-ynyl)-3-[[3-(4-isoxazolyl)phenyl]methoxy]-N-methyl-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



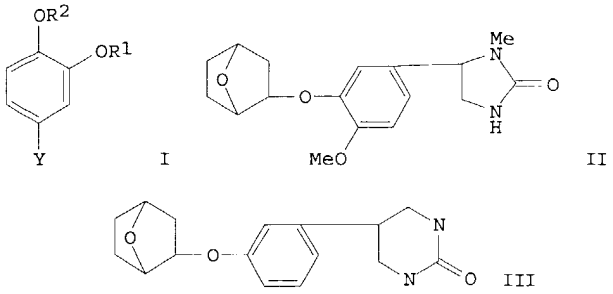
L28 ANSWER 17 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1993:101978 HCAPLUS
DN 118:101978
ED Entered STN: 19 Mar 1993
TI Preparation of aryl substituted nitrogen heterocyclic antidepressants
IN Saccomano, Nicholas A.; Vinick, Fredric J.
PA Pfizer Inc., USA
SO U.S., 28 pp. Division of U.S. Ser. No. 155,932.
CODEN: USXXAM
DT **Patent**
LA English
IC ICM C07D233-30
ICS A61K031-415
NCL 514392000
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	US 5128358	A	19920707	US 1991-696690	19910530	<--
	US 5459145	A	19951017	US 1988-155932	19880119	<--
	US 5196426	A	19930323	US 1992-854136	19920319	<--
	US 5294730	A	19940315	US 1992-984190	19921120	<--
	US 5414127	A	19950509	US 1994-184092	19940119	<--
PRAI	US 1988-155932	A3	19880119	<--		
	US 1991-696690	A3	19910830	<--		
	US 1992-854136	A3	19920319	<--		
	US 1992-984190	A3	19921120	<--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 5128358	ICM	C07D233-30
	ICS	A61K031-415
	NCL	514392000
US 5459145	ECLA	C07C217/60; C07C255/37; C07D233/32; C07D233/42; C07D233/78; C07D239/10B; C07D239/22D1; C07D029/36B; C07D285/08B; C07D285/10B; C07D487/04; C07D487/04 <--

OS MARPAT 118:101978
GI



I II

III

AB Title compds. I (R1 = C7-11 bi-, tricycloalkyl, indan-2-yl; R2 = Me, Et; Y = (substituted) (saturated) 5-6-membered N-containing heterocyclyl), salt, optical isomers, diastereomers, useful as antidepressants (no data), are prepared A mixture of endo- and exo-.alpha.-(methylamino)-3-bicyclo[2.2.1]hept-2-yloxy)-4-methoxybenzeneacetonitrile (preparation given) in THF were treated with 1,1-carbonyldiimidazole, the reaction stirred for 24 h at room temperature, and treated with NaOH, HCl, H2O and saturated salt solution to give endo- and exo-title compound II. Similarly prepared was endo- and exo-title compound III. Addnl. I were prepared

ST aryl heterocycle prepn antidepressant; imidazolidinone polyalkyloxyphenyl prepn antidepressant; thiadiazolidinone bicycloheptyloxyphenyl prepn antidepressant; pyrimidinone bicycloheptyloxyphenyl prepn antidepressant; pyrazole bicycloheptyloxyphenyl prepn antidepressant; imidazopyrimidine bicycloheptyloxyphenyl prepn antidepressant; pyrazolopyrimidine bicycloheptyloxyphenyl prepn antidepressant

IT Antidepressants
(aryl nitrogen heterocycles)

IT 1702-10-9P 10271-43-9P 18684-63-4P, Bicyclo[2.2.2]octan-2-ol
115897-62-6P 115897-63-7P 115897-65-9P 115897-66-0P 115897-69-3P
115897-78-4P 115897-79-5P 115897-81-9P 115897-82-0P 115897-85-3P
115897-86-4P 115897-88-6P 115897-89-7P 115897-91-1P 115897-92-2P
115897-94-4P 115897-95-5P 115897-99-9P **115898-02-7P**
115898-03-8P 115898-04-9P 115898-05-0P 115898-09-4P 115898-10-7P
115898-16-3P 115898-17-4P 115898-18-5P 115898-20-9P 115898-21-0P
115898-37-8P 115898-38-9P 115898-39-0P 115898-42-5P 115898-51-6P
115898-52-7P 115898-54-9P 115898-55-0P 115898-57-2P 115898-58-3P
115898-59-4P 115898-62-9P 115898-63-0P 115898-64-1P 115898-65-2P
115898-66-3P 115898-67-4P 115898-68-5P 115898-69-6P 115898-70-9P
115898-73-2P 115898-74-3P 115898-75-4P 115898-76-5P 115898-77-6P
115898-78-7P 115898-79-8P 131408-40-7P 141184-64-7P 144033-83-0P
144033-84-1P 144033-85-2P 144033-86-3P 144033-87-4P 144033-92-1P
144033-93-2P 144034-08-2P 144034-09-3P 144034-10-6P 144034-11-7P
144034-12-8P 144034-13-9P 144034-14-0P 144034-15-1P 144034-16-2P
144034-17-3P 144034-18-4P 144034-20-8P 144124-74-3P
144365-77-5P 144365-78-6P
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction of, in preparation of antidepressants)

IT 115897-70-6P 115897-71-7P 115897-73-9P 115897-75-1P 115897-77-3P
115897-80-8P 115897-83-1P 115897-84-2P 115897-87-5P 115897-90-0P
115897-93-3P 115897-96-6P 115897-97-7P 115897-98-8P 115898-00-5P
115898-06-1P 115898-07-2P 115898-08-3P 115898-11-8P 115898-12-9P
115898-19-6P 115898-22-1P 115898-29-8P 115898-30-1P 115898-34-5P
115898-36-7P 115919-88-5P 144033-88-5P 144033-89-6P 144033-90-9P
144033-91-0P 144033-94-3P 144033-95-4P 144033-96-5P 144033-97-6P
144033-98-7P 144033-99-8P 144034-00-4P 144034-01-5P 144034-02-6P
144034-03-7P 144034-04-8P 144034-05-9P 144034-06-0P 144034-07-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, antidepressant)

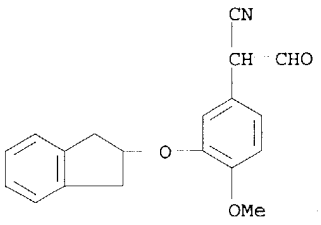
IT 57-13-6, Urea, reactions 64-04-0, Benzeneethanamine 105-53-3, Diethyl malonate 107-11-9, 2-Propen-1-amine 120-80-9, Pyrocatechol, reactions 124-63-0, Methanesulfonyl chloride 302-01-2, Hydrazine, reactions 372-09-8, Cyanoacetic acid 497-36-9 497-38-1, Norcamphor 530-62-1 542-69-8 557-66-4, Ethylaminehydrochloride 621-59-0, Isovanillin 700-57-2, 2-Adamantanol 931-64-6, Bicyclo[2.2.2]oct-2-ene 1820-80-0, 1H-Pyrazol-3-amine 1965-38-4 2534-77-2, exo-2-Bromonorbornane 6160-65-2 6351-10-6, 1-Indanol 7374-90-5 7803-58-9, Sulfamide 13380-89-7 13380-94-4 42383-61-9, 2-Aminoimidazolesulfate 50447-20-6 144034-19-5

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of heterocyclic antidepressants)

IT **115898-02-7P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction of, in preparation of antidepressants)

RN 115898-02-7 HCAPLUS

CN Benzeneacetonitrile, 3-[(2,3-dihydro-1H-inden-2-yl)oxy]-.alpha.-formyl-4-methoxy- (9CI) (CA INDEX NAME)



L28 ANSWER 18 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1991:61950 HCAPLUS

DN 114:61950

ED Entered STN: 23 Feb 1991

TI Preparation and formulation of tetra- and decahydroquinoline-4-carboxylic acids and analogs for use in tissue irrigating solutions

IN Leclerc, Gerard; Ruhland, Beatrice; Andermann, Guy; De Burlet, Georges; Dietz, Michel

PA Laboratoires Alcon S. A., Fr.

SO U.S., 16 pp.
CODEN: USXXAM

DT **Patent**

LA English

IC ICM C07D215-48
ICS A61K031-47

NCL 514311000

CC 27-17 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 63

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 4952573	A	19900828	US 1988-172047	19880323 <--
PRAI US 1988-172047		19880323 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4952573	ICM	C07D215-48
	ICS	A61K031-47
	NCL	514311000

OS CASREACT 114:61950

AB The title compds. having .gamma.-aminobutyric acid (GABA) like activity, were prepared for use in tissue irrigating solns. to promote corneal deswelling during otic surgery. Thus, N-methylquinoline-4-carboxamide was stirred with Ni-Al alloy in aqueous MeOH containing KOH and the product refluxed 14 h with aqueous HCl to give 1,2,3,4-tetrahydroquinoline-4-carboxylic acid-HCl, which gave 34.6 .mu.m reduction of bovine corneal swelling after 3 h perfusion at 0.01 mM compared to 17.2 .mu.m reduction by GABA under the same conditions.

ST quinolinecarboxylate prepn otic tissue irrigant

IT Edema
(corneal, surgery associated, isoquinolinecarboxylates and analogs for prevention of)

IT Eye, disease or disorder
(cornea, surgery associated edema of, quinolinecarboxylates and analogs for prevention of)

IT Pharmaceutical dosage forms
(solns., ophthalmic, irrigation, quinolinecarboxylates and analogs for prevention of surgery-associated corneal edema)

IT **123705-23-7P**
RL: **SPN (Synthetic preparation)**; FORM (Formation, nonpreparative); **PREP (Preparation)**
(formation of, in preparation of otic tissue irrigant)

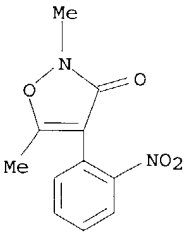
IT 108890-73-9P 123705-20-4P 123705-21-5P **123705-22-6P**
123705-24-8P 123705-25-9P 123705-26-0P
123705-27-1P 123705-28-2P 131753-21-4P **131753-24-7P**
131753-25-8P 131753-26-9P 131753-27-0P 131753-29-2P
131753-30-5P 131753-31-6P 131753-33-8P 131753-34-9P 131753-35-0P
131753-36-1P 131753-37-2P 131753-39-4P 131753-40-7P
131774-41-9P 131774-42-0P
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction of, in preparation of otic tissue irrigant)

IT 13337-72-9P 13337-80-9P 131753-22-5P 131753-23-6P 131753-28-1P
131753-32-7P 131753-38-3P 131753-41-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as otic tissue irrigant)

IT 87-25-2 486-74-8, 4-Quinolinecarboxylic acid 541-41-3,
Ethylchloroformate 2969-81-5 10565-19-2 72802-70-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of otic tissue irrigant)

IT **123705-23-7P**
RL: **SPN (Synthetic preparation)**; **SPN (Synthetic preparation)**; **PREP (Preparation)**
(formation of, in preparation of otic tissue irrigant)

RN 123705-23-7 HCAPLUS
CN 3(2H)-Isoxazolone, 2,5-dimethyl-4-(2-nitrophenyl)- (9CI) (CA INDEX NAME)



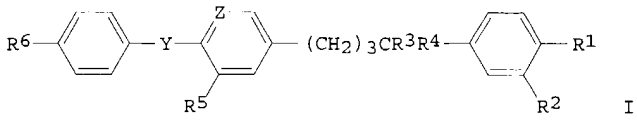
L28 ANSWER 19 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1989:57524 HCAPLUS
DN 110:57524
ED Entered STN: 17 Feb 1989
TI Preparation of 6-pyridyl- and 6-phenyl-3-phenyl-1-hexenes and -1-hexynes as insecticides and acaricides
IN Matsuo, Noritada; Tsushima, Kazunori; Nishida, Sumio; Yano, Toshihiko; Hirano, Masachika
PA Sumitomo Chemical Co., Ltd., Japan
SO U.S., 23 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC ICM A01N043-40
ICS A01N033-10; C07D405-10; C07C149-31
NCL 514717000
CC 27-16 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 5
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 4772633	A	19880920	US 1986-831180	19860220 <--
PRAI US 1986-831180		19860220 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4772633	ICM	A01N043-40
	ICS	A01N033-10; C07D405-10; C07C149-31
	NCL	514717000

OS CASREACT 110:57524; MARPAT 110:57524
GI



I

AB The title compds. (I; R1, R2 = H, halo, alkyl, CF3, alkoxy, alkenyloxy, haloalkoxy; R1R2 = OCH2O; R3 = CH:CH, C.tplbond.C; R4 = H, alkyl; R5 = H, F; R6 = H, halo, alkyl, alkoxy, CF3; Y = O, S, CH2, NH; Z = N, CH) were prepared 4-(EtO)C6H4CH2CN was stirred 1 h at -50.degree. with (Me2CH)2NLi in THF whereupon MeI was added and stirring continued 13 h to give 4-(EtO)C6H4CHMeCN which was stirred 30 min with NaH in DMF, 3-(PhO)C6H4(CH2)3Br added, and stirring continued 12 h to give 3-(PhO)C6H4(CH2)3CMe(CN)C6H4(OEt)-4. The latter was reduced with Dibal in PhMe to the corresponding aldehyde which was added to Ph3PMeBr in THF previously stirred with BuLi and the mixture stirred 14 h to give 3-(PhO)C6H4(CH2)3CMe(CH:CH2)C6H4(OEt)-4 which caused .gtoreq.90% mortality to Culex pipiens pallens larvae at 3.5 ppm in aqueous solution

ST pyridylphenylhexene hexyne prepn insecticide acaricide; hexene hexyne diphenyl prepn insecticide acaricide

IT Acaricides
Insecticides
(pyridylphenyl- and diphenylhexenes and -hexynes)

IT 51558-05-5P, 2-(4-Ethoxyphenyl)propionitrile 105128-01-6P 105128-02-7P
105128-03-8P 105128-04-9P 105128-05-0P **105128-06-1P**
105128-07-2P 105128-08-3P 105128-09-4P 105128-10-7P 105128-14-1P
105128-15-2P 118365-86-9P 118365-87-0P 118365-88-1P 118365-89-2P
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction of, in preparation of insecticides and acaricides)

IT 105127-61-5P 105127-62-6P 105127-63-7P 105127-64-8P 105127-65-9P
105127-66-0P 105127-67-1P 105127-68-2P 105127-69-3P 105127-70-6P
105127-71-7P 105127-72-8P 105127-73-9P 105127-74-0P 105127-75-1P
105127-76-2P 105127-77-3P 105127-78-4P 105127-79-5P 105127-80-8P
105127-81-9P 105127-82-0P 105127-83-1P 105127-84-2P 105127-85-3P
105127-86-4P 105127-87-5P 105127-88-6P 105127-89-7P 105127-90-0P
105127-91-1P 105127-92-2P 105127-93-3P 105127-94-4P 105127-95-5P
105127-97-7P 105127-98-8P 105127-99-9P 105147-96-4P 105147-97-5P
105147-98-6P 105147-99-7P 118383-67-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as insecticide and acaricide)

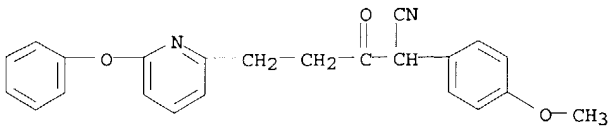
IT 104-47-2, 4-Methoxyphenylacetonitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of insecticides and acaracides)

IT 5927-18-4, Trimethylphosphonoacetate 6775-77-5, 4-Ethoxyphenylacetonitrile 68523-22-8, 2-Formyl-6-phenoxypyridine 105128-00-5, 3-(3-Phenoxyphenyl)propylbromide 105128-13-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of insecticides and acaricides)

IT **105128-06-1P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction of, in preparation of insecticides and acaricides)

RN 105128-06-1 HCAPLUS

CN 2-Pyridinepentanenitrile, .alpha.-(4-methoxyphenyl)-.beta.-oxo-6-phenoxy- (9CI) (CA INDEX NAME)



L28 ANSWER 20 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1987:63041 HCAPLUS
DN 106:63041
ED Entered STN: 07 Mar 1987
TI Synergistic insecticidal compositions containing dione esters
IN Sousa, Anthony A.

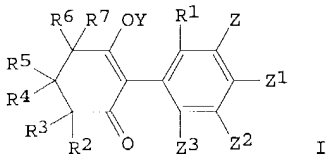
PA Union Carbide Corp., USA
SO U.S., 17 pp. Cont. of U.S. Ser. No. 277,731, abandoned.
CODEN: USXXAM
DT **Patent**
LA English
IC ICM A01N037-34
ICS A01N053-00
NCL 514521000
CC 5-4 (Agrochemical Bioregulators)
Section cross-reference(s): 25
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4613617	A	19860923	US 1985-724960	19850423 <--

PRAI US 1981-277731 19810626 <--
CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4613617	ICM	A01N037-34
	ICS	A01N053-00
	NCL	514521000

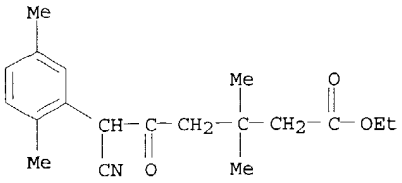
OS CASREACT 106:63041
GI



I

AB Dione ester derivs. I [Z, Z1, Z2, Z3 = H, haloalkyl, polyhaloalkyl, halo, alkyl, alkoxy, cyano, NO2, alkylthio, alkylsulfinyl, alkylsulfonyl, alkanoyl, CONH2, NH2; Y = COR; R = H, halo, (un)substituted alkyl, alkenyl, alkynyl, bicycloalkyl, bicycloalkenyl, cycloalkyl, cycloalkenyl, Ph, phenylalkyl, naphthyl, naphthylalkyl; R1 = alkyl, polyhaloalkyl, haloalkyl, halo; R2, R3, R4, R5, R6, R7 = H, (un)substituted alkyl, Ph, cyano, halo, NO2, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, dialkylamino, etc.] are prepared as insecticides. I are synergistic with known insecticides. Thus, 2.0 g 2-ethylhexanoyl chloride was added to a solution of 1.50 g 2-(2',4'-dimethylphenyl)-5,5-dimethyl-1,3-cyclohexanedione and 1.94 g pyridine in 10 mL CHCl3. The mixture was stirred for 2 h at room temperature, then refluxed for 12 h to give 1.15 g 3-(2-ethylhexanoyloxy)-5,5-dimethyl-2-(2',4'-dimethylphenyl)-2-cyclohexenone (II). II and carbaryl synergistically kill the housefly (Musca domestica).
ST cyclohexenone prepn synergistic insecticide
IT Insecticides
(synergistic, phenylcyclohexenone-containing compns.)
IT 108-67-8, Mesitylene, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with diazocyclohexanedione)
IT 126-81-8, 5,5-Dimethyl-1,3-cyclohexanedione
RL: BIOL (Biological study)
(condensation of, with dichloronitrobenzene)
IT 99-54-7, 3,4-Dichloronitrobenzene 20098-48-0, 3,4,5-Trichloronitrobenzene
RL: BIOL (Biological study)
(condensation of, with dimethylcyclohexanedione)
IT 1460-08-8, 2-Diazocyclohexane-1,3-dione
RL: BIOL (Biological study)
(condensation of, with mesitylene)
IT 1807-68-7, 2-Diazo-5,5-dimethylcyclohexane-1,3-dione
RL: BIOL (Biological study)
(condensation of, with xylene)
IT 68427-57-6 68429-54-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of)
IT 760-67-8, 2-Ethylhexanoyl chloride
RL: BIOL (Biological study)
(esterification with (chlorophenyl)dimethylcyclohexanedione)
IT 142-61-0, Hexanoyl chloride
RL: BIOL (Biological study)

(esterification with (dimethylphenyl)dimethylcyclohexanedione)
IT 298-00-0, Methyl parathion 35400-43-2, Sulprofos 51630-58-1
52645-53-1, Permethrin 52918-63-5, Decamethrin
RL: BIOL (Biological study)
(insecticidal composition containing, synergized by dione ester)
IT 108-88-3, Toluene, biological studies
RL: BIOL (Biological study)
(photoreaction of, with diazodecalindione)
IT 98-19-1
RL: BIOL (Biological study)
(photoreaction of, with diazodimethylcyclohexanedione)
IT 68427-55-4P 68427-57-6P 68427-58-7P **68427-60-1P**
68427-62-3P 68427-63-4P **101582-73-4P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and cyclocondensation of)
IT 68427-39-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deamination of)
IT 68427-40-7P 68427-41-8P 68427-43-0P 68427-44-1P 68427-45-2P
68427-46-3P 68427-47-4P 68427-49-6P 68427-50-9P 68427-52-1P
68427-56-5P 68427-59-8P 68427-61-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of)
IT 68427-51-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and photoreaction of, with toluene)
IT 68427-48-5P, 2-Diazo-5-phenylcyclohexane-1,3-dione
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with mesitylene)
IT 68427-38-3P 68427-42-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
IT 68427-64-5P 68427-65-6P 68427-67-8P 68427-68-9P 68427-69-0P
68428-15-9P 72619-67-1P 83786-58-7P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as insecticide)
IT 16213-85-7 68429-53-8, 2,4-Dimethylbenzylcyanide
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with di-Et dimethylglutarate)
IT 108-38-3, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with diazocyclohexanedione derivative, in synthesis of insecticides)
IT 17804-59-0, Diethyl 3,3-dimethylglutarate
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with dimethylbenzyl cyanide)
IT 941-55-9, Tosyl azide
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phenylcyclohexanedione)
IT 493-72-1, 5-Phenylcyclohexane-1,3-dione 68429-52-7, Decalin-1,3-dione
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with tosyl azide)
IT **68427-60-1P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and cyclocondensation of)
RN 68427-60-1 HCAPLUS
CN Benzenehexanoic acid, .epsilon.-cyano-.beta.,.beta.,2,5-tetramethyl-.delta.-oxo-, ethyl ester (9CI) (CA INDEX NAME)



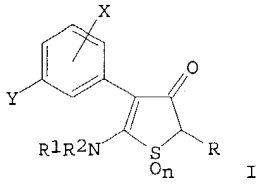
L28 ANSWER 21 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1986:552917 HCAPLUS
DN 105:152917
ED Entered STN: 01 Nov 1986
TI Herbicidal 5-amino-3-oxo-4-(substituted phenyl)-2,3-dihydrothiophenes and their derivatives
IN Ward, Carl E.
PA Chevron Research Co. , USA
SO U.S., 22 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC ICM A01N043-02
ICS A01N043-40; A01N043-36; C07D333-16
NCL 071090000
CC 27-8 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 5
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4596595	A	19860624	US 1984-623805	19840622 <--
	WO 8702220	A1	19870423	WO 1985-US2004	19851011 <--
	W: AT, AU, BR, CH, DE, GB, JP, KR, NL				
	AU 8548672	A1	19870505	AU 1985-48672	19851011 <--
	AU 593224	B2	19900208		
	NL 8520343	A	19870901	NL 1985-20343	19851011 <--
	BR 8507300	A	19871103	BR 1985-7300	19851011 <--
	DE 3590848	T	19871210	DE 1985-3590848	19851011 <--
	JP 63501073	T2	19880421	JP 1985-504754	19851011 <--
	CH 673651	A	19900330	CH 1987-2274	19851011 <--
	AT 8509085	A	19930115	AT 1985-90	19851011 <--
	AT 396470	B	19930927		
	CA 1280752	A1	19910226	CA 1985-493921	19851025 <--
	IL 76882	A1	19920329	IL 1985-76882	19851030 <--
	FR 2590253	A1	19870522	FR 1985-17064	19851119 <--
	FR 2590253	B1	19880212		
	GB 2191191	A1	19871209	GB 1987-9948	19870427 <--
	GB 2191191	B2	19890913		
PRAI	US 1984-623805		19840622 <--		
	WO 1985-US2004		19851011 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4596595	ICM	A01N043-02
	ICS	A01N043-40; A01N043-36; C07D333-16
	NCL	071090000

OS CASREACT 105:152917
GI



AB The title compds. [I; R = (halo)alkyl, cycloalkyl, (cycloalkyl)alkyl, (halo)alkenyl, alkoxy, alkylthio, alkoxyalkyl, 4-FC6H4, (un)substituted Ph, naphthyl, indenyl, substituted arylmethyl; R1 = H, C1-4 alkyl; R2 = H,

C1-4 alkyl, C3-4 alkenyl, alkoxycarbonylalkyl, alkoxyalkyl, alkylthioalkyl; R1R2N = heterocyclyl; X = H, alkyl, alkoxy, halo, CF3; Y = alkyl, alkoxy, halo, haloalkyl, haloalkoxy, haloalkylthio; n = 0-2] and their salts, useful as herbicides and plant growth regulators, were prepared Thus, MeSCH2COCH(C6H4CF3-3)CN in THF was treated with (Me3Si)2NLi and MeI to give MeCH(SMe)COCH(C6H4CF3-3)CN ,which was cyclized in AcOH with H2SO4 to give I (R = Me; R1 = R2 = X = H; Y = CF3 ; n = 0) (II). In preemergence tests, II at 27.5 .mu.g/cm2 was 100% phytotoxic to lambsquarter and crab- and watergrass with no damage to wild oats and rice.

ST aminophenylthiophenone prepn herbicide plant growth regulator; thiophenone aminophenyl prepn herbicide

IT Herbicides
(aminophenyldihydrothiophenones and their oxides)

IT Plant hormones and regulators
RL: RCT (Reactant); RACT (Reactant or reagent)
(aminophenyldihydrothiophenones and their oxides)

IT Molecular structure-biological activity relationship
(herbicidal, of aminophenyldihydrothiophenones and their oxides)

IT 101-97-3 104456-12-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with acetonitrile derivative)

IT 2338-76-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with phenylacetates)

IT 104456-10-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(homologation of)

IT **104456-09-9P 104456-11-3P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and cyclization of, thiophene from)

IT **68084-26-4P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and cyclization of, with sulfur, thiophene from)

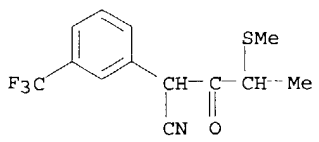
IT 18729-76-5P 18729-77-6P 104456-64-6P 104456-65-7P 104456-66-8P
104456-67-9P 104456-68-0P 104456-69-1P 104456-70-4P 104456-71-5P
104456-72-6P 104456-73-7P 104456-74-8P 104456-75-9P 104456-76-0P
104456-77-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and herbicidal activity of)

IT 104456-08-8P 104456-13-5P 104456-14-6P 104456-15-7P 104456-16-8P
104456-17-9P 104456-18-0P 104456-19-1P 104456-20-4P 104456-21-5P
104456-22-6P 104456-23-7P 104456-24-8P 104456-25-9P 104456-26-0P
104456-27-1P 104456-28-2P 104456-29-3P 104456-30-6P 104456-31-7P
104456-32-8P 104456-33-9P 104456-34-0P 104456-35-1P 104456-36-2P
104456-37-3P 104456-38-4P 104456-39-5P 104456-40-8P 104456-41-9P
104456-42-0P 104456-43-1P 104456-44-2P 104456-45-3P 104456-46-4P
104456-47-5P 104456-48-6P 104456-49-7P 104456-50-0P 104456-51-1P
104456-52-2P 104456-53-3P 104456-54-4P 104456-55-5P 104456-56-6P
104456-57-7P 104456-58-8P 104456-59-9P 104456-60-2P 104456-61-3P
104456-62-4P 104456-63-5P 104456-78-2P 104471-83-2P 104471-84-3P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as herbicide and plant growth regulator)

IT **104456-09-9P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and cyclization of, thiophene from)

RN 104456-09-9 HCAPLUS

CN Benzeneacetonitrile, .alpha.-[2-(methylthio)-1-oxopropyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



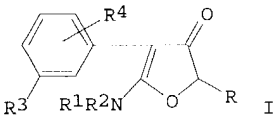
L28 ANSWER 22 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1986:420517 HCAPLUS
DN 105:20517
ED Entered STN: 26 Jul 1986
TI Herbicidal 5-amino-3-oxo-4-(substituted-phenyl)-2,3-dihydrofuran
IN Ward, Carl E.
PA Chevron Research Co. , USA
SO U.S., 14 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC ICM A01N043-08
ICS C07D307-66
NCL 071088000
CC 5-3 (Agrochemical Bioregulators)
Section cross-reference(s): 27
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 4568377	A	19860204	US 1985-727459	19850426 <--
PRAI US 1985-727459		19850426 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4568377	ICM	A01N043-08
	ICS	C07D307-66
	NCL	071088000

OS CASREACT 105:20517
GI



I

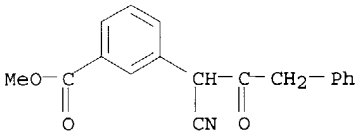
AB The title compds. I [R = (un)substituted Ph, naphth-1-yl, inden-1-yl; R2 = H, alkyl; R2 = H, alkyl, alkenyl, alkoxythioalkyl, etc.; NR1R2 = ring; R3 = CN, NO2, alkoxycarbonyl, etc.; R4 = H, halo, alkyl, alkoxy, F3C] are herbicides. Thus, pre-emergence I (R = Ph, R1 = R4 = H, R2 = Me, R3 = CO2Et) (27.5 .mu.g/cm2) totally controlled lambsquaters, mustard, crabgrass, and other weeds, in pot expts. I are prepared by cyclization of the corresponding acylacetonitriles.
ST furanone herbicide prepn
IT Herbicides
(aminooxophenyldihdyrofurans)
IT 68432-92-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation of)
IT 103-80-0
RL: BIOL (Biological study)
(condensation of, with methoxycarbonylphenylacetyl)
IT 101480-90-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(methylation of)
IT **101480-83-5P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and cyclization of)
IT 23145-00-8P 23145-02-0P 76996-63-9P 96541-91-2P 96541-92-3P
96541-93-4P 96541-94-5P 96541-95-6P 96541-96-7P 96541-97-8P
96572-49-5P 96572-50-8P 96572-51-9P 96906-18-2P 96906-20-6P
96906-21-7P 101480-84-6P 101480-85-7P 101480-88-0P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as herbicide)
IT 101480-86-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, with herbicide)
IT 106-95-6, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with (fluorophenyl)oxo(methoxycarbonylphenyl)methylaminodihydrofuran)

IT 101480-87-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with early bromide)

IT **101480-83-5P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and cyclization of)

RN 101480-83-5 HCAPLUS
CN Benzoic acid, 3-(1-cyano-2-oxo-3-phenylpropyl)-, methyl ester (9CI) (CA INDEX NAME)



L28 ANSWER 23 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1986:420516 HCAPLUS
DN 105:20516
ED Entered STN: 26 Jul 1986
TI 2-Substituted 5-amino-3-oxo-4-(substituted-phenyl)-2,3-dihydrofuran herbicides
IN Ward, Carl E.
PA Chevron Research Co. , USA
SO U.S., 13 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC ICM A01N043-08
ICS C07D307-52
NCL 071088000
CC 5-3 (Agrochemical Bioregulators)
Section cross-reference(s): 27

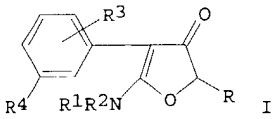
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 4568375	A	19860204	US 1984-666075	19841026 <--
PRAI US 1984-666075		19841026 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4568375	ICM	A01N043-08
	ICS	C07D307-52
	NCL	071088000

OS CASREACT 105:20516
GI



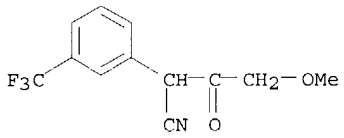
I

AB The herbicidal title compds. I (R = halo, alkoxy, alkenylmethoxy; R1 = alkyl; R2 = alkyl, alkenyl, alkoxycarbonylalkyl, etc.; NR1R2 = ring; R3 = H, alkyl, halo, etc.; R4 = alkyl, haloalkyl, etc.) are prepared by halogenation of I (R = H) with a N-halosuccinimide, under UV light, followed eventually by alkylation. Thus, a solution of I (R = R3 = H, R1 = R2 = Me, R4 = 3-F3C(C6H4) (preparation given), N-bromosuccinimide and a small amount of Bz2O2 in C6H6 was irradiated with 300-600 nm light for 2 h, to give I (R = Br, R1 = R2 = Me, R3 = H, R4 = 3-F3(C6H4) which was reacted with EtONa, to give I (R = OEt, R1 = R2 = Me, R3 = H, R4 = F3C) (II). In pot expts., pre-emergence 27.5 .mu.g II/cm2 totally controlled crabgrass, wild oats, lambsquaters, mustard, and other weeds.

ST furanone herbicide prepn; halogenation furanone UV light

IT Halogenation

(of phenyldimethylaminodihydrofuranones, photochem.)
IT Herbicides
(phenylaminodihydrofuranones)
IT 101480-91-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and bromination of)
IT **96541-98-9P**
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and cyclization of)
IT 101480-92-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and epoxylation of)
IT 96525-52-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and methylation)
IT 23145-00-8P 23145-02-0P 76996-63-9P 96541-91-2P 96541-92-3P
96541-93-4P 96541-94-5P 96541-95-6P 96541-96-7P 96541-97-8P
96572-49-5P 96572-50-8P 96572-51-9P 96906-18-2P 96906-20-6P
96906-21-7P 101480-93-7P 101480-94-8P 101480-95-9P 101480-96-0P
101480-97-1P 101480-98-2P 101504-44-3P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as herbicide)
IT **96541-98-9P**
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and cyclization of)
RN 96541-98-9 HCAPLUS
CN Benzeneacetonitrile, .alpha.-(methoxyacetyl)-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



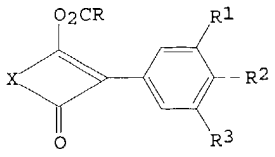
L28 ANSWER 24 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1986:19417 HCAPLUS
DN 104:19417
ED Entered STN: 24 Jan 1986
TI Biocidal enol esters of non-ortho substituted 2-aryl-1,3-cycloalkanedione compounds
IN Wheeler, Thomas N.; Weiden, Mathias H. J.
PA Union Carbide Corp. , USA
SO U.S., 10 pp. Cont. of U.S. Ser. No. 946,311 abandoned.
CODEN: USXXAM
DT **Patent**
LA English
IC ICM C11C003-04
ICS C07C069-03
NCL 260410500
CC 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 5
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 4526723	A	19850702	US 1983-510731	19830705 <--
PRAI US 1978-946311		19780927 <--		

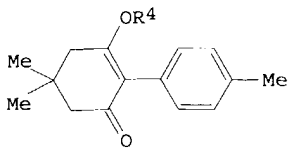
CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4526723	ICM	C11C003-04
	ICS	C07C069-03
	NCL	260410500

OS CASREACT 104:19417
GI



I



II

AB Title compds. I [R = (un)substituted alkyl, alkenyl, alkynyl, Ph, haloalkyl, cycloalkyl, cycloalkenyl, phenylalkyl; R1, R2, R3 = H, haloalkyl, halo, alkyl; X = (un)substituted C2, C3 alkylene], useful as acaricides and herbicides, were prepared Thus, Et 3,3-dimethylglutarate reacted with 4-MeC6H4CH2CN to give 68% 4-MeC6H4CH(CN)COCH2CMe2CH2CO2Et, which cyclized to give 57% of the enol II (R4 = H). The last was treated with Me(CH2)6COCl to give II [R4 = CO(CH2)6Me] (III). At 2500 ppm preemergent, III gave complete inhibition of crabgrass (Digitaria sanguinalis) without damage to the tomatoes. III also gave excellent control of 2-spotted mites (Tetranychus urticae) as adults and eggs.

ST acaricide arylcycloalkanedione enol ester prepn; herbicide arylcycloalkanedione enol ester prepn; arylcycloalkanedione enol ester acaricide herbicide; cycloalkanedione enol ester acaricide herbicide

IT Acaricides
Herbicides
(arylcycloalkanedione enol esters)

IT Enols
RL: RCT (Reactant); RACT (Reactant or reagent)
(esters of, of arylcycloalkanediones, as acaricides and herbicides)

IT Esters, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(of arylcycloalkanedione enols, preparation and acaricidal and herbicidal activity of)

IT **99480-51-0P 99480-53-2P**
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and cyclization of, to cyclohexanedione)

IT 99480-52-1P 99480-54-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of, with alkanoyl chloride)

IT 83786-58-7P 83786-59-8P 83786-60-1P 83786-61-2P 83786-62-3P
83786-63-4P 83786-67-8P 99480-38-3P 99480-39-4P 99480-40-7P
99480-41-8P 99480-42-9P 99480-43-0P 99480-44-1P 99480-45-2P
99480-46-3P 99480-47-4P 99480-48-5P 99480-49-6P 99480-50-9P
99480-55-4P 99480-56-5P 99480-57-6P 99480-58-7P 99480-59-8P
99496-99-8P 99497-00-4P 99497-01-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, acaricidal, and herbicidal activity of)

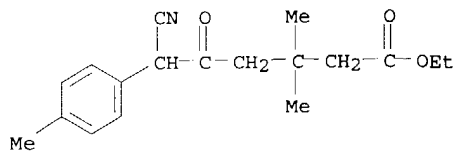
IT 17804-59-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with benzyl cyanide)

IT 1529-41-5 2947-61-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with glutarate)

IT **99480-51-0P**
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and cyclization of, to cyclohexanedione)

RN 99480-51-0 HCAPLUS

CN Benzenehexanoic acid, .epsilon.-cyano-.beta.,.beta.,4-trimethyl-.delta.-oxo-, ethyl ester (9CI) (CA INDEX NAME)



L28 ANSWER 25 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1985:6812 HCAPLUS

DN 102:6812

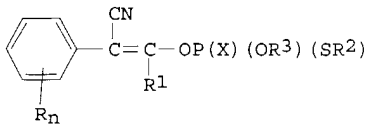
ED Entered STN: 12 Jan 1985
TI Pesticidal cyano enol phosphates
IN D'Silva, Themistocles D. J.
PA Union Carbide Corp. , USA
SO U.S., 9 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC A01N057-14; C07F009-165
NCL 424210000
CC 29-7 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 5
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 4469688	A	19840904	US 1982-393552	19820630 <--
PRAI US 1982-393552		19820630 <--		

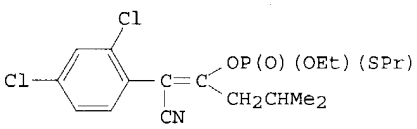
CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4469688	IC	A01N057-14IC C07F009-165
	NCL	424210000

OS CASREACT 102:6812
GI



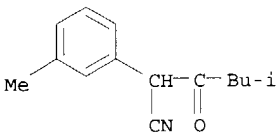
I



II

AB About 29 title compds. I [R = H, alkyl, alkylthio, alkoxy, trihalomethyl, di- or trifluoromethoxy, halo; R1 = H, (un)substituted alkyl, halocycloalkyl, alkenyl, alkenylcycloalkyl, alkynyl, trihaloalkyl, alkoxycarbonyl, PhCH2, alkyl, alkoxyalkyl, haloalkoxyalkyl, alkoxycarbonylalkyl, alkoxyphenyl, haloalkoxyphenyl, alkoxycarbonylphenyl; X = O; n = 0-5; R2 = Pr, R3 = Et], insecticides and miticides, were prepared Thus, treating 2,4-Cl2C6H3CH(CN)C(O)CH2CHMe2 in MeCN with ClP(O)(OEt)(SPr) gave 68% thiophosphate (II). Some examples of I were more effective against the two-spotted mite than Kelthane.
ST cyano enol phosphate insecticide; miticide cyano enol phosphate
IT Acaricides
Insecticides
(cyano enol phosphates)
IT 93502-43-3P 93502-44-4P 93502-45-5P 93502-46-6P 93502-47-7P
93502-48-8P 93502-49-9P 93502-50-2P 93502-51-3P 93502-52-4P
93502-53-5P 93502-54-6P 93502-55-7P 93502-56-8P 93502-57-9P
93502-58-0P 93502-59-1P 93502-60-4P 93502-61-5P 93502-62-6P
93502-63-7P 93502-64-8P 93502-65-9P 93502-66-0P 93502-67-1P
93502-68-2P 93502-69-3P 93502-70-6P 93502-71-7P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and pesticidal activity of)
IT **93502-72-8P 93502-73-9P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction with Et Pr chlorothiophosphate)
IT 71871-79-9 93502-74-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with Et Pr chlorothiophosphate)
IT 22364-68-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with Et benzoate)
IT 2947-60-6
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with Et isovalerate)
IT 7651-98-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with acyl-substituted benzyl cyanides)
IT 93-89-0 108-64-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methylbenzyl cyanide)
IT **93502-72-8P**
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction with Et Pr chlorothiophosphate)
RN 93502-72-8 HCAPLUS
CN Benzeneacetonitrile, 3-methyl-.alpha.-(3-methyl-1-oxobutyl)- (9CI) (CA INDEX NAME)



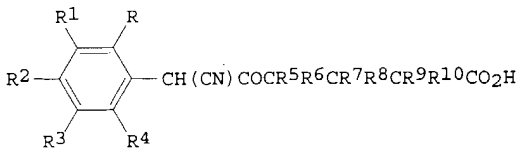
L28 ANSWER 26 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1984:610574 HCAPLUS
DN 101:210574
TI Condensation of substituted phenylacetonitriles with dicarboxylic anhydrides
IN Ligon, Robert C.
PA Union Carbide Corp. , USA
SO U.S., 3 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC C07C121-76
NCL 260465000D
CC 23-16 (Aliphatic Compounds)
Section cross-reference(s): 25
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 4470929	A	19840911	US 1983-480733	19830331 <--
PRAI US 1983-480733		19830331 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4470929	IC	C07C121-76
	NCL	260465000D

GI



I

AB 6-Cyano-6-phenyl-5-oxohexanoic acids I [R = alkyl, halo, polyhaloalkyl, haloalkyl; R1, R2, R3, and R4 are H, NO2, polyhaloalkyl, halo, cyano, alkyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, alkanoyl, amino, haloalkyl; R5, R6, R7, R8, R9, and R10 are H, alkyl, Ph, alkyl-, cyano-, halo-, nitro-, alkoxy-, alkylthio-, alkylsulfinyl-, alkylsulfonyl-, or (dialkylamino)phenyl] were prepared from glutaric anhydrides, phenylacetonitriles, and bases. 3,3-Dimethylglutaric anhydride was heated with 2-MeC6H4CH2CN and NaNH2-NaOCMe3 in THF-Me3COH to give 2-MeC6H4CH(CN)COCH2CMe2CH2CO2H.
ST cyanophenyloxohexanoic acid; hexanoic acid cyano oxo phenyl; condensation glutaric anhydride catalyst; glutaric anhydride condensation phenylacetonitrile
IT Condensation reaction catalysts

(sodium alkoxides, for glutaric anhydride derivative with phenylacetonitrile derivative)

IT 865-48-5
RL: CAT (Catalyst use); USES (Uses)
(catalysts from sodamide and, for condensation of glutaric anhydride derivative with phenylacetonitrile derivative)

IT 7782-92-5
RL: CAT (Catalyst use); USES (Uses)
(catalysts from sodium tert-butoxide and, for condensation of glutaric anhydride derivative with phenylacetonitrile derivative)

IT 141-52-6
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for condensation of glutaric anhydride derivative with phenylacetonitrile derivative)

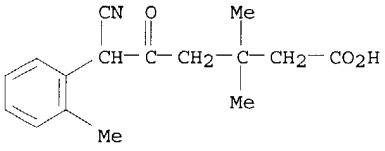
IT 22364-68-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with glutaric anhydride derivative, catalysts for)

IT 4160-82-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with phenylacetonitrile derivative, catalysts for)

IT **93079-58-4P**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of)

IT **93079-58-4P**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of)

RN 93079-58-4 HCAPLUS
CN Benzenehexanoic acid, .epsilon.-cyano-.beta.,.beta.,2-trimethyl-.delta.-oxo- (9CI) (CA INDEX NAME)



L28 ANSWER 27 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1984:610572 HCAPLUS
DN 101:210572
TI Condensation of ring-substituted phenylacetonitriles with monoesters of dicarboxylic acids
IN Ligon, Robert C.
PA Union Carbide Corp. , USA
SO U.S., 3 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC C07C121-76
NCL 260465000D
CC 23-16 (Aliphatic Compounds)
Section cross-reference(s): 25

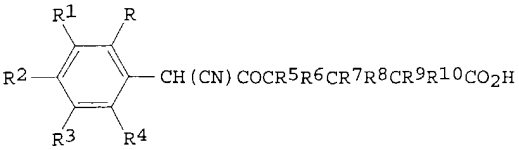
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 4469642	A	19840904	US 1983-480726	19830331 <--
PRAI US 1983-480726		19830331 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4469642	IC	C07C121-76
	NCL	260465000D

GI



I

AB The base-catalyzed reaction of phenylacetonitriles with monoalkyl glutarates gave hexanoic acids I [R = alkyl, halo, polyhaloalkyl, haloalkyl; R1, R2, R3, and R4 are H, NH3, polyhaloalkyl, halo, cyano, alkyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, alkanoyl, amino, haloalkyl; R5, R6, R7, R8, R9, and R10 are H, alkyl, substituted alkyl, Ph, alkyl-, cyano-, halo-, nitro-, alkoxy-, (alkylthio)-, (alkylsulfinyl)-, (alkylsulfonyl)-, or (dialkylamino)phenyl]. Thus, 2-MeC6H4CH2CN underwent a condensation reaction with EtO2CCH2CMe3CH2CO2H and NaOEt to give I (R = R7 = R8 = Me, R1 = R2 = R3 = R4 = R5 = R6 = R9 = R10 = H).

ST butyric acid phenylcyanoacetyl; cyanophenylacetylbutyric acid; phenylcyanoacetylbutyric acid

IT Condensation reaction catalysts
(sodium ethoxide, for phenylacetonitrile derivative with monoethyl glutarate derivative)

IT 141-52-6
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for condensation of phenylacetonitrile derivative with monoethyl glutarate derivative)

IT 22364-68-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with monoethyl glutarate derivative, catalysts for)

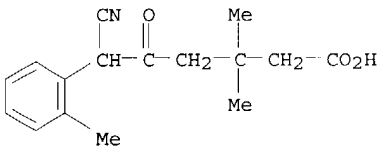
IT 93218-34-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with phenylacetonitrile derivative, catalysts for)

IT **93079-58-4P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)

IT **93079-58-4P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)

RN 93079-58-4 HCAPLUS

CN Benzenehexanoic acid, .epsilon.-cyano-.beta.,.beta.,2-trimethyl-.delta.-oxo- (9CI) (CA INDEX NAME)



L28 ANSWER 28 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1982:544457 HCAPLUS

DN 97:144457

ED Entered STN: 12 May 1984

TI Biocidal 2-aryl-1,3-cyclopentanedione compounds and their alkali metal and ammonium salts

IN Wheeler, Thomas N.

PA Union Carbide Corp. , USA

SO U.S., 16 pp. Cont.-in-part of U.S. 4,283,348.
CODEN: USXXAM

DT **Patent**

LA English

IC A61K031-12; C07C049-427; A01N031-00

NCL 071122000

CC 24-4 (Alicyclic Compounds)
Section cross-reference(s): 5

FAN.CNT 2

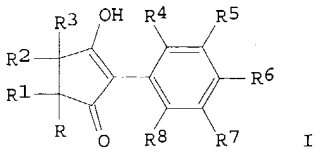
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 4338122	A	19820706	US 1980-197600	19801016 <--
US 4283348	A	19810811	US 1979-78923	19790926 <--
PRAI US 1978-944995		19780922	<--	
US 1979-78923		19790926	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4338122	IC	A61K031-12IC C07C049-427IC A01N031-00
	NCL	071122000

OS CASREACT 97:144457

GI



I

AB Title compds. I [R, R1, R2, and R3 individually are H, (un)substituted alkyl, alkenyl, cycloalkyl, cycloalkenyl, or Ph, or any two of R, R1, R2, and R3 form an alkylene or alkenylene bridge; R4 = alkyl, haloalkyl, halo; R5, R6, R7, and R8 individually are H, NO2, haloalkyl, halo, cyano, alkyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, alkanoyl, amino] were prepared, and they exhibited herbicidal and acaricidal activity. Thus, 2,4-Cl2C6H3CH2CN was acylated by EtO2CCH2CH2CO2Et, the product was converted to 2,4-Cl2C6H3CH2COCH2CH2CO2Et, and the latter was heated with Na in EtOH to give 2-(2,4-dichlorophenyl)-1,3-cyclopentanedione.

ST phenylcyclopentanedione prepn herbicide acaricide; cyclopentanedione phenyl prepn herbicide

IT Acaricides
Herbicides
(phenylcyclopentanediones and perhydroindandione analogs)

IT 4676-51-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation by, of phenylacetonitrile derivative)

IT 123-25-1 10138-59-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation by, of phenylacetonitriles)

IT 6306-60-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation of, by succinate ester)

IT 22364-68-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation of, by succinate ester derivative)

IT 16213-85-7 68429-53-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation of, by succinate esters)

IT 83190-41-4
RL: PROC (Process)
(addition of, with benzaldehyde derivative)

IT 874-42-0
RL: PROC (Process)
(addition of, with bicyclooctenone derivative)

IT 80036-04-0P 83190-40-3P 83190-42-5P 83190-43-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion of, to indandione derivative)

IT 80035-92-3P 80035-98-9P 80035-99-0P 80036-08-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclocondensation of)

IT 80035-91-2P 80035-96-7P 80035-97-8P 80036-07-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of, by ethanol)

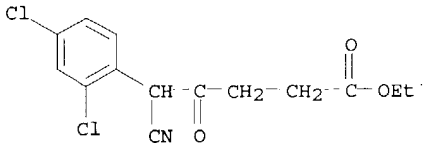
IT 80035-93-4P 80036-00-6P 80036-03-9P 80036-05-1P 80036-09-5P
80036-11-9P 80036-14-2P 80036-15-3P 80036-16-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and herbicidal and acaricidal activity of)

IT **80035-90-1P 80035-94-5P 80035-95-6P**
80036-01-7P 80036-06-2P 80036-10-8P
80036-13-1P
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and hydrolysis-decarboxylation of)

IT **80035-90-1P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and hydrolysis-decarboxylation of)

RN 80035-90-1 HCAPLUS

CN Benzenepentanoic acid, 2,4-dichloro-.delta.-cyano-.gamma.-oxo-, ethyl ester (9CI) (CA INDEX NAME)



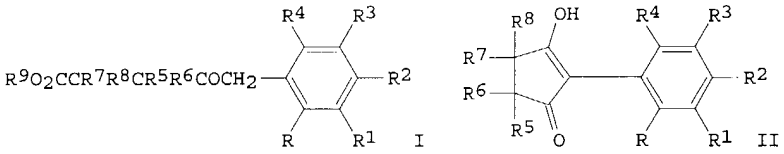
L28 ANSWER 29 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1982:6260 HCAPLUS
DN 96:6260
ED Entered STN: 12 May 1984
TI 2-Aryl-1,3-cyclopentanedione compounds
IN Wheeler, Thomas N.
PA Union Carbide Corp. , USA
SO U.S., 12 pp. Division of U.S. Ser. No. 944,995.
CODEN: USXXAM
DT **Patent**
LA English
IC C07C049-707; C07C121-76; C07C147-10
NCL 260465000D
CC 24-4 (Alicyclic Compounds)
Section cross-reference(s): 5, 25
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4283348	A	19810811	US 1979-78923	19790926 <--
	US 4338122	A	19820706	US 1980-197600	19801016 <--
PRAI	US 1978-944995		19780922	<--	
	US 1979-78923		19790926	<--	

CLASS

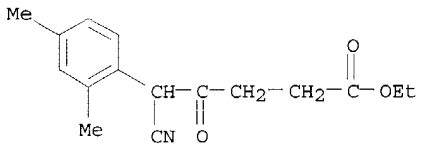
PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES		
US 4283348	IC	C07C049-707IC	C07C121-76IC	C07C147-10
	NCL	260465000D		

OS CASREACT 96:6260
GI



AB 4-Oxopentanoate esters I [R = alkyl, haloalkyl, halo, polyhaloalkyl; R1, R2, R3, and R4 individually are H, NO2, polyhaloalkyl, halo, cyano, alkyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, alkanoyl, amino, haloalkyl; R5, R6, R7, and R8 individually are H, (un)substituted alkyl, alkenyl, cycloalkyl, or cycloalkenyl, Ph, alkyl-, alkanoyl-, cycloalkyl-, cycloalkenyl-, cyano-, halo-, nitro-, alkoxy-, aryloxy-, alkylthio-, arylthio-, alkylsulfinyl-, alkylsulfonyl-, (acylamino)-, or (dialkylamino)phenyl; R9 = alkyl] were treated with NaOEt at 100-25.degree. to yield title compds. II, which exhibited acaricidal and herbicidal activity. Thus, 2,4-Cl2C6H3CH2CN was acylated by EtO2CCH2CH2CO2Et and the product was converted to EtO2CCH2CH2COCH2C6H3Cl2-2,4 (III) in two steps, and III (in PhMe) was heated with Na in EtOH at .apprx.100.degree. to give 2-(2,4-dichlorophenyl)-1,3-cyclopentanedione.
ST phenylcyclopentanedione prepn acaricide herbicide; cyclopentanedione phenyl prepn herbicide
IT Acaricides
Herbicides
(phenylcyclopentanediones and phenylhexahydroindanones)
IT 123-25-1 10138-59-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation of phenylacetonitriles by)
IT 22364-68-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation of, by diethylsuccinate derivative)

IT 4676-51-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation of, by phenylacetonitrile derivative)
IT 6306-60-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation of, by succinate ester)
IT 16213-85-7 68429-53-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation of, by succinate ester derivs.)
IT 36461-33-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(addition reaction of, with benzaldehyde derivative)
IT 874-42-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(addition reaction of, with cyclobutenediol disilyl ether derivative)
IT 80035-93-4P 80036-00-6P 80036-03-9P 80036-05-1P 80036-09-5P
80036-11-9P 80036-14-2P 80036-15-3P 80036-16-4P 80036-17-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and acaricidal and herbicidal activity of)
IT 80035-92-3P 80035-98-9P 80035-99-0P **80036-06-2P**
80036-08-4P
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and cyclocondensation reaction of)
IT 80035-91-2P 80035-96-7P 80035-97-8P 80036-07-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of, by ethanol)
IT **80035-90-1P 80035-94-5P 80035-95-6P**
80036-01-7P 80036-10-8P 80036-13-1P
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and hydrolysis of, decarboxylation in)
IT 80036-02-8P 80036-04-0P 80036-12-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and rearrangement of indandione analog from)
IT **80036-06-2P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and cyclocondensation reaction of)
RN 80036-06-2 HCAPLUS
CN Benzenepentanoic acid, .delta.-cyano-2,4-dimethyl-.gamma.-oxo-, ethyl ester (9CI) (CA INDEX NAME)



L28 ANSWER 30 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1981:603926 HCAPLUS
DN 95:203926
ED Entered STN: 12 May 1984
TI Substituted isoxazolines for control of plant phytopathogens
IN Davenport, James D.
PA Eli Lilly and Co., USA
SO U.S., 5,668, abandoned.
CODEN: USXXAM
DT **Patent**
LA English
IC C07D413-04; A01N043-80
NCL 424263000
CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 5
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4283403	A	19810811	US 1977-829304	19770831 <--
	IL 51948	A1	19800630	IL 1977-51948	19770426 <--
	CA 1082185	A1	19800722	CA 1977-277139	19770427 <--
	GB 1581583	A	19801217	GB 1977-24189	19770609 <--

BE 855602	A1	19771212	BE 1977-8185	19770610	<--
JP 52153959	A2	19771221	JP 1977-70432	19770613	<--
FR 2355010	A1	19780113	FR 1977-18050	19770613	<--
FR 2355010	B1	19800201			
BR 7703803	A	19780418	BR 1977-3803	19770613	<--
NL 7706558	A	19771216	NL 1977-6558	19770614	<--
BR 7703863	A	19780425	BR 1977-3863	19770614	<--
CH 627049	A	19811231	CH 1977-7307	19770614	<--

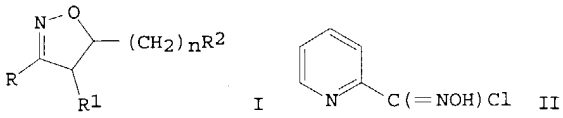
PRAI US 1976-695668 19760614 <--

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4283403	IC	C07D413-04IC A01N043-80
	NCL	424263000

OS CASREACT 95:203926

GI



I II

AB 2-Isoxazolines I (R = 2-pyridyl; R1 = H, Ph; n = 1, 2; R2 = isothiocyanato) were prepared and exhibited fungicidal activity. Thus, treating imidoyl chloride II, prepared from the aldoxime, with CH2:CHCH2NCS and Et3N gave I (R = 2-pyridyl, R1 = H, n = 1, R2 = isothiocyanato). Similarly prepared were I (R = Ph, alkoxy-, nitro-, alkyl-, or halophenyl; R1 = H, Ph; n = 1, 2; R2 = isothiocyanato, cyano, NH2) which also showed fungicidal activity.

ST isoxazoline isothiocyanatomethyl prepn fungicide; isothiocyanatomethylisoxazoline prepn fungicide

IT Fungicides and Fungistats
((isothiocyanatoalkyl)isoxazolines)

IT 110-91-8, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(addition reaction of, with (isothiocyanatoalkyl)isoxazolines)

IT 74-89-5, reactions 108-18-9 302-01-2, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(addition reaction of, with (isothiocyanatomethyl)isoxazoline derivs.)

IT 932-90-1
RL: PROC (Process)
(conversion of, to N-hydroxybenzamidoyl chloride)

IT 459-23-4 3235-02-7 25185-95-9 34158-73-1 56843-28-8
RL: PROC (Process)
(conversion of, to N-hydroxybenzimidoyl chloride derivative)

IT 3235-04-9
RL: PROC (Process)
(conversion of, to N-hydroxybenzimidoyl chlorides)

IT 873-69-8
RL: PROC (Process)
(conversion of, to N-hydroxyimidoyl chloride analog)

IT 3717-28-0 29203-59-6 65788-66-1 65788-68-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(cycloaddn. reaction of, with allyl isothiocyanate)

IT 109-75-1 19364-21-7 65788-85-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(cycloaddn. reaction of, with N-hydroxybenzimidoyl chloride)

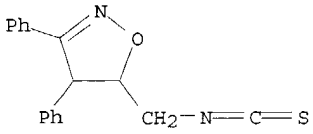
IT 2253-93-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(cycloaddn. reaction of, with N-hydroxybenzimidoyl chlorides)

IT 57-06-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(cycloaddn. reaction of, with N-hydroxybenzimidoyl chlorides, isoxazolines from)

IT 104-88-1, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(oximation of)

IT 122-03-2 454-89-7 455-19-6 555-16-8, reactions 3218-36-8 6502-22-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(oximation of, and conversion of product to N-hydroxybenzimidoyl chloride derivative)

IT 4397-53-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(oximation of, and conversion of products to N-hydroxybenzimidoyl chlorides)
IT 3848-36-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion of, to N-hydroxybenzimidoyl chloride derivative)
IT 698-16-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and cycloaddn. reaction of, with alkenyl isothiocyanates, allyl cyanide and allylamine derivs.)
IT 42202-94-8P 42202-95-9P 61946-90-5P 65788-87-6P 65788-96-7P
69716-28-5P 79754-91-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cycloaddn. reaction of, with allyl isothiocyanate)
IT 1011-84-3P 6579-27-7P 28123-63-9P 29203-60-9P 33126-97-5P
36288-37-6P 38435-51-7P 69053-93-6P 74467-05-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cycloaddn. reaction of, with aryl isothiocyanate)
IT 6501-74-2P 14654-87-6P 65788-61-6P 65788-62-7P 65788-63-8P
65788-64-9P 65788-67-2P 65788-69-4P 65788-70-7P 65788-71-8P
65788-72-9P 65788-73-0P 65788-74-1P 65788-75-2P 65788-76-3P
65788-77-4P 65788-78-5P 65788-79-6P 65788-80-9P 65788-81-0P
65788-82-1P 65788-83-2P **65788-86-5P** 65788-88-7P
65788-92-3P 65788-93-4P 65788-94-5P 65788-95-6P 65991-25-5P
79754-92-0P 79754-93-1P 79754-94-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); **SPN (Synthetic preparation)**; BIOL (Biological study); **PREP (Preparation)**
(preparation and fungicidal activity of)
IT **65788-86-5P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); **SPN (Synthetic preparation)**; BIOL (Biological study); **PREP (Preparation)**
(preparation and fungicidal activity of)
RN 65788-86-5 HCAPLUS
CN Isoxazole, 4,5-dihydro-5-(isothiocyanatomethyl)-3,4-diphenyl- (9CI) (CA INDEX NAME)



L28 ANSWER 31 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1981:84125 HCAPLUS
DN 94:84125
ED Entered STN: 12 May 1984
TI Substituted arylcyanoalkyl and diaryl cyanoalkylimidazoles
IN Miller, George A.; Chan, Hak-Foon; Carley, Harold E.
PA Rohm and Haas Co., USA
SO U.S., 18 pp. Cont.-in-part of U.S. 4,143,137.
CODEN: USXXAM
DT **Patent**
LA English
IC C07D233-90
NCL 548341000
CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 5
FAN.CNT 4

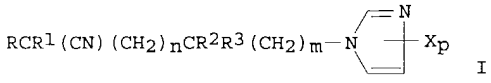
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4225723	A	19800930	US 1979-1658	19790108 <--
	US 4073921	A	19780214	US 1976-647039	19760107 <--
	CA 1067903	A1	19791211	CA 1976-244896	19760203 <--
	CH 621777	A	19810227	CH 1976-1354	19760204 <--
	AT 7600810	A	19791115	AT 1976-810	19760205 <--
	AT 357365	B	19800710		
	PL 107215	P	19800229	PL 1976-187683	19760303 <--

	PL 123447	B1	19821030	PL 1976-200363	19760303 <--
	US 4143137	A	19790306	US 1977-839877	19771006 <--
	FR 2384761	A1	19781020	FR 1978-4787	19780220 <--
	FR 2384761	B1	19800829		
PRAI	US 1975-557546		19750312 <--		
	US 1976-647039		19760107 <--		
	US 1977-839877		19771006 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4225723	IC	C07D233-90
	NCL	548341000

GI



I

AB 1-Unsubstituted imidazoles were N-alkylated by arylcyanoalkyl halides and mesylates and NaH, NaOH, or quaternary ammonium halides to yield 1-(arylcyanoalkyl)imidazoles I [R = aryl, halo-, nitro-, cyano-, alkoxy-, alkyl-, (trihalomethyl)-, benzyl-, or phenylaryl, or CRR1 = fluorenylidene; R1 = alkyl, cycloalkyl, alkenyl, cycloalkenyl, alkynyl, Ph, halo-, nitro-, cyano-, alkoxy-, alkyl-, or (trihalomethyl)phenyl, (un)substituted benzyl, (un)substituted phenethyl; n = 0, 1, 2, 3, 4, 5; R2 and R3 are independently H, alkyl, Ph, halo-, nitro-, cyano-, alkoxy-, alkyl-, or (trihalomethyl)phenyl, (un)substituted benzyl, (un)substituted phenethyl; m = 0, 1, 2, 3, 4, 5; p = 0, 1, 2 (X = halo)], which showed fungicidal activity. Thus, 2,4-Cl2C6H3CHBuCN was hydroxymethylated by paraformaldehyde, the product was converted to 2-cyano-2-(2,4-dichlorophenyl)hexyl mesylate (II), and imidazole reacted with II to give I (n = m = p = 0, R = 2,4-Cl2C6H3, R1 = Bu, R2 = R3 = H).

ST arylcyanoalkylimidazole prepn fungicide; imidazole arylcyanoalkyl prepn fungicide

IT Fungicides and Fungistats
(N-(phenylcyanoalkyl)imidazoles)

IT 89-98-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of, with bromochlorobenzene)

IT 106-39-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of, with chlorobenzaldehyde)

IT 61019-78-1P 61019-79-2P 61019-81-6P 61019-82-7P 61019-83-8P
61019-85-0P 61019-86-1P 61019-87-2P 61019-88-3P 61019-89-4P
61019-90-7P 61019-91-8P 61019-92-9P 61019-93-0P 61019-94-1P
61019-96-3P 61023-03-8P 61023-04-9P 61023-05-0P 61023-06-1P
61023-09-4P 61023-10-7P 61023-11-8P 61023-12-9P 61023-13-0P
61023-15-2P 61023-17-4P 61023-18-5P 61023-19-6P 61023-20-9P
61023-21-0P 61023-22-1P 61023-24-3P 61023-26-5P 61023-28-7P
61023-30-1P 61023-31-2P 61023-33-4P 61023-34-5P 61023-35-6P
61023-36-7P 61023-37-8P 61023-38-9P 61023-39-0P 61023-40-3P
61023-41-4P 61023-42-5P 61023-43-6P 61023-44-7P 61023-45-8P
61023-46-9P 61023-92-5P 61055-47-8P 61055-49-0P 61055-50-3P
76562-08-8P 76562-10-2P 76562-11-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and fungicidal activity of)

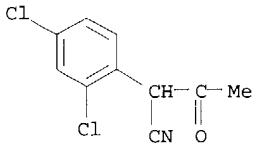
IT 43171-49-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with phosphorus tribromide)

IT 61023-86-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and substitution reaction of, with cuprous cyanide)

IT 3508-98-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and .alpha.-chloromethylation of)

IT 58830-59-4P 58830-64-1P 59666-80-7P 61023-87-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation and .alpha.-hydroxymethylation of)
IT 61023-79-8P 61023-82-3P 61023-84-5P 61023-88-9P 61023-90-3P
61023-93-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(preparation and O-mesylation of)
IT 76562-14-6P **76562-15-7P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)
IT 61023-80-1P 61023-81-2P 61023-83-4P 61023-85-6P 61023-89-0P
61023-91-4P 61023-94-7P 76562-12-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, and N-alkylation of imidazole by)
IT 20968-04-1P 58830-65-2P 63866-57-9P 76562-13-5P 76562-16-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, for N-alkylation of imidazole)
IT 140-29-4 6306-60-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(.alpha.-alkylation of)
IT 109-69-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(.alpha.-alkylation of phenylacetonitrile by)
IT 103-63-9 111-24-0 111-83-1 542-69-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(.alpha.-alkylation of phenylacetonitrile derivative by)
IT 75-09-2, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(.alpha.-chloromethylation of phenylacetonitrile derivative by)
IT 2184-88-5 5005-36-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(.alpha.-hydroxymethylation of)
IT 30525-89-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(.alpha.-hydroxymethylation of phenylacetonitriles by)
IT 288-32-4, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(N-alkylation of, by phenylalkyl mesylates)
IT **76562-15-7P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)
RN 76562-15-7 HCAPLUS
CN Benzeneacetonitrile, .alpha.-acetyl-2,4-dichloro- (9CI) (CA INDEX NAME)

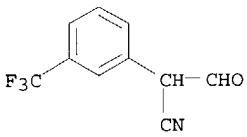


L28 ANSWER 32 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1981:30760 HCAPLUS
DN 94:30760
ED Entered STN: 12 May 1984
TI Substituted 6-phenyl-1,2,4-triazolo[4,3-a]pyridines
IN Albright, Jay D.; Trust, Ronald I.
PA American Cyanamid Co., USA
SO U.S., 11 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC C07D471-04; A61K031-44
NCL 546119000
CC 28-11 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 27
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 4209626	A	19800624	US 1979-20886	19790315 <--
PRAI US 1979-20886		19790315 <--		

CLASS
PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES

(Reactant or reagent)
(preparation and decarboxylation of)
IT 76053-48-0P 76053-49-1P 76053-50-4P 76066-36-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrazinolysis of)
IT 76066-49-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenation of)
IT 35982-93-5P 35982-98-0P 59198-14-0P 76053-34-4P 76053-35-5P
76053-36-6P 76053-37-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
IT 15131-89-2P 19927-64-1P 59198-06-0P 76053-33-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with cyanoacetamide)
IT 76053-41-3 76053-42-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation decarboxylation of)
IT 2338-76-3P 10177-08-9P **70806-40-5P** 76053-40-2P 76053-45-7P
76053-47-9P 76066-42-7P 76066-43-8P 76066-44-9P 76066-45-0P
76066-46-1P 76066-48-3P 76066-51-8P 76066-52-9P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)
IT 64-19-7, reactions 331-25-9 351-35-9 1878-66-6 2444-36-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with DMF)
IT 109-94-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with benzeneacetonitrile derivative)
IT 68-12-2, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phenylacetates)
IT **70806-40-5P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)
RN 70806-40-5 HCAPLUS
CN Benzeneacetonitrile, .alpha.-formyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L28 ANSWER 33 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1980:568298 HCAPLUS
DN 93:168298
ED Entered STN: 12 May 1984
TI (Substituted-phenyl)-1,2,4-triazolo[4,3-a]pyrimidines and (substituted-phenyl)-1,2,4-triazolo[1,5-a]pyrimidines
IN Albright, Jay D.; Dusza, John P.; Hardy, Robert A., Jr.
PA American Cyanamid Co., USA
SO U.S., 12 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC A61K031-505; C07D487-04
NCL 544263000
CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
FAN.CNT 1

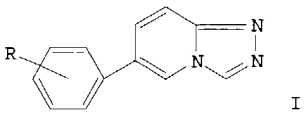
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 4209621	A	19800624	US 1979-34060	19790427 <--
PRAI US 1979-34060		19790427 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES

US 4209626	IC	C07D471-04IC	A61K031-44
	NCL	546119000	

GI



I

AB Triazolopyridines I (R = H, C1-4 alkyl, C1-4 alkoxy, F, Cl, Br, CF3, cyano, CO2H, C2-5 alkoxycarbonyl, CONH2, NO2, NH2, AcNH, C1-4 alkylamino, dialkylamino), useful as antihypertensives (no data), were prepared Thus, 4-ClC6H4C(CHO):CHNMe2, prepared by the condensation of DMF and 4-ClC6H4CH2CO2H in the presence of POCl3, was cyclocondensed with NCCH2CONH2, hydrolyzed, decarboxylated, chlorinated by POCl3, and hydrazinolyzed to give 5-(4-chlorophenyl)-2-hydrazinopyridine (II). The cyclocondensation of II and HC(OEt)3 gave I (R = 4-Cl).

ST propenal phenylamino prepn cyclocondensation cyanoacetamide; hydrazinophenylpyridine prepn cyclocondensation orthoformate; pyridine hydrazinophenyl prepn cyclocondensation orthoformate; malonamide phenylpropenal cyclocondensation; formylhydrazine chlorophenylpyridine cyclocondensation; triazolopyridine prepn antihypertensive

IT Antihypertensives
(phenyl-1,2,4-triazolo[4,3-a]pyridines)

IT 108-59-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with aminophenylpropenal)

IT 108-59-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with aminopnenylpropenal)

IT 624-84-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with chloro(chlorophenyl)pyridine)

IT 53868-37-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with cyanoacetamide)

IT 22252-94-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with di-Me malonate)

IT 76066-36-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with formylhydrazine)

IT 107-91-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with phenyl(dimethylamino)propenals)

IT 122-51-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with phenylhydrazinopyridines)

IT 105-53-3 108-13-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with phenylpropenal derivative)

IT 66600-05-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrazinolysis of)

IT 76066-47-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis of)

IT 76053-43-5P 76053-44-6P 76053-46-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and chlorination of)

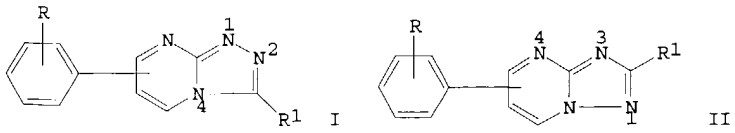
IT 76066-37-0P 76066-38-1P 76066-39-2P 76066-40-5P 76066-41-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclocondensation of, with Et orthoformate)

IT 76066-50-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclocondensation of, with di-Me malonate)

IT 10177-08-9P 76053-38-8P 76053-39-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

US 4209621 IC A61K031-505IC C07D487-04
NCL 544263000

GI



AB 2-Hydrazinopyrimidines underwent a cyclocondensation reaction with ortho esters to give triazolo[4,3-a]pyrimidines I (R = Cl, F, CF3, alkoxy; R1 = H, alkyl), and triazolo[1,5-a]pyrimidines II (R and R1 same as above) were prepared by the reaction of .beta.-aminoacrylophenones with 3-amino-1,2,4-triazole; I and II are useful as anxiolytic agents (no data). A mixture of 2-hydrazino-5-phenylpyrimidine and HC(OEt)3 was refluxed 16 h to give 6-phenyl-[1,2,4]triazolo[4,3-a]pyrimidine.

ST phenyltriazolopyrimidine prepn anxiolytic; triazolopyrimidine phenyl prepn anxiolytic

IT Anxiety
(phenyltriazolopyrimidines effect on)

IT 99-02-5 99-91-2 100-06-1 349-76-8 403-42-9 445-27-2 586-37-8 2142-68-9 17408-14-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction of, with DMF di-Me acetal)

IT 4637-24-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction of, with acetophenones)

IT 1201-93-0 1717-42-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation reaction of, with aminotriazole)

IT 35260-96-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation reaction of, with hydrazine)

IT 78-39-7 115-80-0 122-51-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation reaction of, with hydrazinopyrimidines)

IT 57-13-6, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation reaction of, with .alpha.-(iminomethyl)phenylacetaldehydes, pyrimidines from)

IT 4923-01-7 22819-05-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation reaction of, with .beta.-aminoacrylophenone derivative)

IT 62-56-6, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation reaction of, with .beta.-aminoacrylophenones)

IT 61-82-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation reactions of, with (aminomethylene)phenylacetaldehydes and .beta.-aminoacrylophenones)

IT 62041-46-7P 72851-51-5P 75175-76-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclocondensation reaction of, with aminotriazole)

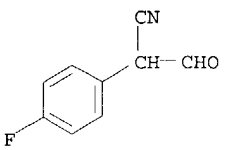
IT 72851-19-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclocondensation reaction of, with aminotriazoles)

IT 71734-79-7P 75175-43-8P 75175-44-9P 75175-46-1P 75175-47-2P 75175-48-3P 75175-49-4P 75175-50-7P 75175-90-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclocondensation reaction of, with ortho esters)

IT 75175-45-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclocondensation reaction of, with orthoacetate ester)

IT 51777-47-0P 75175-26-7P 75175-27-8P 75175-28-9P 75175-29-0P 75175-30-3P 75175-31-4P 75175-32-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cyclocondensation reaction of, with urea)
IT 27956-39-4P 56863-46-8P 74963-17-0P 75175-33-6P 75175-35-8P
75175-36-9P 75175-37-0P 75175-38-1P 75175-84-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with phosphoryl chloride)
IT 75175-85-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reductive dechlorination of)
IT **398-42-5P 5841-70-3P 62538-21-0P**
66154-58-3P 70806-40-5P 75175-23-4P
75175-24-5P 75175-25-6P
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and selective hydrogenation of)
IT 22536-62-5P 27956-40-7P 56734-11-3P 74963-13-6P 75175-39-2P
75175-40-5P 75175-41-6P 75175-42-7P 75175-89-2P 75185-49-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and substitution reaction of, with hydrazine)
IT 2338-75-2P 2338-76-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and .alpha.-formylation of)
IT 60414-59-7P 75175-87-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and S-methylation of)
IT 56734-10-2P 75175-88-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and S-oxidation of)
IT 3038-47-9P 18096-70-3P 28587-05-5P 39573-72-3P 63680-91-1P
72851-21-9P 72851-22-0P 75175-34-7P 75175-51-8P 75175-52-9P
75175-53-0P 75175-54-1P 75175-55-2P 75175-56-3P 75175-57-4P
75175-58-5P 75175-59-6P 75175-60-9P 75175-61-0P 75175-62-1P
75175-63-2P 75175-64-3P 75175-65-4P 75175-66-5P 75175-67-6P
75175-68-7P 75175-69-8P 75175-70-1P 75175-71-2P 75175-72-3P
75175-73-4P 75175-74-5P 75175-75-6P 75175-77-8P 75175-78-9P
75175-79-0P 75175-80-3P 75175-81-4P 75175-82-5P 75175-83-6P
75175-86-9P 75175-91-6P 75175-92-7P 75175-93-8P 75175-94-9P
75175-95-0P 75175-96-1P 75185-50-1P 75185-51-2P 75185-52-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 302-01-2, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution reaction of, with chloropyrimidines)
IT 395-44-8 402-23-3 402-49-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution reaction of, with potassium cyanide)
IT 109-94-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(.alpha.-acylation of phenylacetonitriles by)
IT 140-29-4 140-53-4 459-22-3 501-00-8 1529-41-5 2856-63-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(.alpha.-formylation of)
IT 74-88-4, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(S-alkylation of pyrimidinethiols by)
IT **398-42-5P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and selective hydrogenation of)
RN 398-42-5 HCAPLUS
CN Benzeneacetonitrile, 4-fluoro-.alpha.-formyl- (9CI) (CA INDEX NAME)



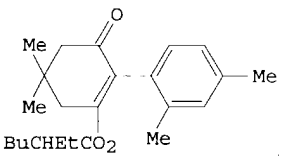
L28 ANSWER 34 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1980:400924 HCAPLUS
DN 93:924
ED Entered STN: 12 May 1984
TI Controlling acarina ectoparasites on warmblooded animals by orally administering to the animal an ectoparasitically-effective amount of a 2-aryl-1,3-cyclohexanedione compound, and alkali metal salts, ammonium salts and enol esters
IN Haines, Robert G.
PA Union Carbide Corp., USA
SO U.S., 17 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC A61K031-22; A61K031-12; A61K031-275
NCL 424311000
CC 1-5 (Pharmacodynamics)
Section cross-reference(s): 25
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4175135	A	19791120	US 1978-925814	19780718 <--
	ZA 7903507	A	19800730	ZA 1979-3507	19790712 <--
	AU 7948939	A1	19800124	AU 1979-48939	19790716 <--
	AU 529257	B2	19830602		
	DK 7902990	A	19800119	DK 1979-2990	19790717 <--
	EP 7243	A1	19800123	EP 1979-301409	19790717 <--
	EP 7243	B1	19821117		
	R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
	AT 1813	E	19821215	AT 1979-301409	19790717 <--
	FI 7902259	A	19800119	FI 1979-2259	19790718 <--
	CA 1150626	A1	19830726	CA 1979-332184	19790719 <--
PRAI	US 1978-925814		19780718 <--		
	EP 1979-301409		19790717 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES		
US 4175135	IC	A61K031-22IC	A61K031-12IC	A61K031-275
	NCL	424311000		

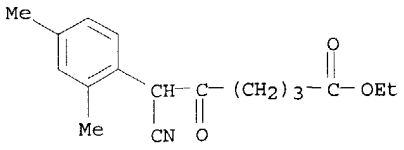
GI



I

AB 2-Aryl-1,3-cyclohexanediones are effective against ticks when given orally. Thus, 3-(2-ethylhexanoyloxy)-5,5-dimethyl-2(2',4'-dimethylphenyl)-2-cyclohexenone (I) [68427-67-8] was effective against Dermacentor variabilis, Amblyomma americanum, and Amblyomma maculatum when given orally to sheep at 7.0 mg/kg/day.
ST arylcyclohexanedione tick
IT Acaricides
(arylcyclohexanediones as)
IT 68427-46-3 72619-67-1 72619-68-2
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)
(acaricidal activity of)
IT 68429-54-9 72619-69-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of)
IT 493-72-1 68429-52-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(diazotization of)
IT 30581-70-5DP, aryl derivs. 68427-67-8P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and acaricidal activity of)
IT 68427-39-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and chlorination of)
IT 68427-43-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deamination of)
IT **68429-55-0P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and hydrolysis of)
IT 68427-48-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with mesitylene)
IT 68427-51-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with toluene)
IT 68427-38-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
IT 68427-39-4P 68427-40-7P 68427-41-8P 68427-42-9P 68427-44-1P
68427-46-3P 68427-47-4P 68427-49-6P 68427-50-9P 68427-52-1P
68427-53-2P 68427-55-4P 68427-56-5P 68427-57-6P
68427-59-8P **68427-60-1P** 68427-61-2P 68427-62-3P
68427-64-5P 68427-65-6P 68427-66-7P 68427-68-9P 68427-69-0P
71885-47-7P
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of)
IT 760-67-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chlorophenyldimethylcyclohexanedione)
IT 108-67-8, biological studies
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with diazocyclohexanedione)
IT 126-81-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with dichloronitrobenzene)
IT 1460-08-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with mesitylene)
IT 1807-68-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with xylene)
IT **68429-55-0P**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 68429-55-0 HCAPLUS
CN Benzenehexanoic acid, .epsilon.-cyano-2,4-dimethyl-.delta.-oxo-, ethyl ester (9CI) (CA INDEX NAME)



L28 ANSWER 35 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1978:546892 HCAPLUS
DN 89:146892
ED Entered STN: 12 May 1984
TI Isoxazolines
IN Duranleau, Roger G.
PA Texaco Inc., USA
SO U.S., 4 pp.
CODEN: USXXAM
DT **Patent**

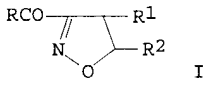
LA English
IC C07D261-20
NCL 260307000DA
CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 40
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4092327	A	19780530	US 1976-738996	19761105 <--
PRAI	US 1976-738996		19761105 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4092327	IC	C07D261-20
	NCL	260307000DA

GI



I

AB Isoxazolines I (R = C1-20 alkyl, aryl; R1, R2 = H, C1-18 alkyl, C2-18 alkylene, aryl or R1R2 = polymethylene) were prepared by cyclocondensation of R1CH:CHR2 with RCOCH2NO2. Thus, Me(CH2)5CH:CH2 and Me(CH2)11COCH2NO2 heated at reflux in PhMe containing p-MeC6H4SO3H 7.5 h gave I [R = Me(CH2)11, R1 = H, R2 = hexyl]. I were useful as intermediates for photog. sensitizers.

ST isoxazoline acyl alkyl; alkanone isoxazolinyl

IT Alkenes, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with .alpha.-nitro ketones)

IT Cyclocondensation reaction
(of alkenes with .alpha.-nitro ketones)

IT Ketones, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(.alpha.-nitro, cyclocondensation of, with alkenes)

IT 10230-68-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with 1,2-diphenylethylene)

IT 55601-76-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with 1-octene)

IT 54044-25-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with 2-pentene)

IT 13291-54-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with cyclohexene)

IT 100-42-5, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with nitroacetophenone)

IT 109-68-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with nitrodecanone)

IT 110-83-8, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with nitrohexadecanone)

IT 588-59-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with nitropropanone)

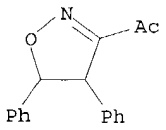
IT 111-66-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with nitrotetradecanone)

IT 614-21-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with styrene)

IT 7064-02-0P 67743-77-5P **67743-78-6P** 67743-79-7P 67743-80-0P
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of)

IT **67743-78-6P**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of)

RN 67743-78-6 HCAPLUS
CN Ethanone, 1-(4,5-dihydro-4,5-diphenyl-3-isoxazolyl)- (9CI) (CA INDEX NAME)



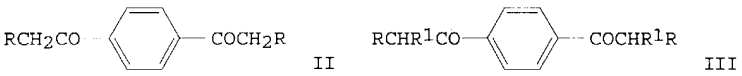
L28 ANSWER 36 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1977:584219 HCAPLUS
DN 87:184219
ED Entered STN: 12 May 1984
TI 1,4-Bis(arylacetyl)benzenes
IN Harris, Frank W.; Reinhardt, Bruce A.
PA Wright State University, USA
SO U.S., 5 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC C07C049-76
NCL 260590000E
CC 25-16 (Noncondensed Aromatic Compounds)
Section cross-reference(s): 27
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 4046814	A	19770906	US 1975-641959	19751218 <--
PRAI US 1975-641959		19751218 <--		

CLASS

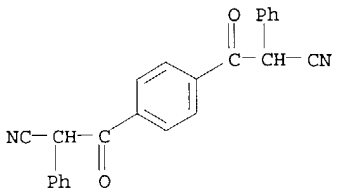
PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 4046814	IC	C07C049-76
	NCL	260590000E

GI



AB Terephthalic acid (I) derivs. were converted to diketones II (R = Ph, 2-pyridyl). I di-Me ester condensed with PhCH2CN and the III (R = Ph, R1 = CN) product was hydrolyzed and decarboxylated to give II (R = Ph). III (R = 2-pyridyl, R1 = CO2Et), which was prepared from I acid chloride and Et (2-pyridyl)acetate, was saponified and decarboxylated to yield II (R = 2-pyridyl).
ST benzyl phenyl ketone; pyridylmethyl phenyl ketone; benzene bisarylacetyl
IT 140-29-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction of, with dimethyl terephthalate)
IT 100-20-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction of, with ethyl pyridylacetate)
IT 120-61-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction of, with phenylacetonitrile)
IT 2739-98-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction of, with terephthaloyl dichloride)
IT 3363-92-6P 64549-34-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **64549-33-3P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation, hydrolysis and decarboxylation of)
IT 64549-35-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, saponification and decarboxylation of)

IT **64549-33-3P**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation, hydrolysis and decarboxylation of)
RN 64549-33-3 HCAPLUS
CN 1,4-Benzenedipropanenitrile, .beta.,.beta.'-dioxo-.alpha.,.alpha.'-diphenyl- (9CI) (CA INDEX NAME)



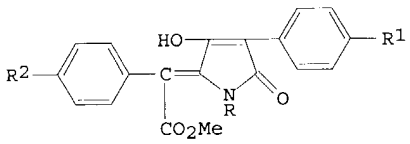
L28 ANSWER 37 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1977:55276 HCAPLUS
DN 86:55276
ED Entered STN: 12 May 1984
TI Compositions comprising tetramic acid analogs of pulvinic acid for combating arthritis
IN Weinstock, Joseph
PA Smithkline Corp., USA
SO U.S., 12 pp. Division of U.S. 3,931,207.
CODEN: USXXAM
DT **Patent**
LA English
IC A61K031-40
NCL 424263000
CC 27-10 (Heterocyclic Compounds (One Hetero Atom))
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3984559	A	19761005	US 1975-623226	19751017 <--
	US 3931207	A	19760106	US 1973-424581	19731214 <--
PRAI	US 1973-424581		19731214 <--		

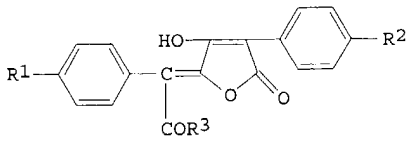
CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3984559	IC	A61K031-40
	NCL	424263000

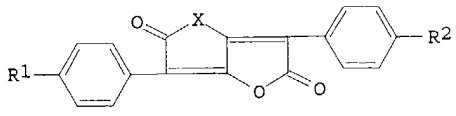
GI



I



II



III

AB Tetramic acid derivs. I (R = 2-thiazolyl, 2-pyridyl, 5-chloro-2-pyridyl, 3-pyridyl, R1 = R2 = H; R = 2-thiazolyl, R1 = R2 = Cl; R = R2 = H, R1 = Me) were prepared by treating 4-R1C6H4CH2CN with (EtO2C)2, treating 4-R1C6H4CH(CN)COCO2Et with 4-R2C6H4CH2CN, cyclizing 4-

R1C6H4CH(CN)COCOCH(CN)C6H4R2-4 with acid, cyclizing II (R3 = OH) with Ac2O, treating III (X = O) with RNH2, cyclizing II (R3 = NHR), and methanolysis of III (X = NR).

ST tetramic acid benzylidene; benzylidenetetramic acid; thiazolyltetramic acid carboxybenzylidene; pyridyltetramic acid carboxybenzylidene; arthritis tetramic acid

IT Arthritis
(tetramic acid derivs. in treatment of)

IT 140-29-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with ethyl oxalate)

IT 95-92-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with phenylacetonitriles)

IT **10471-29-1P** 26548-70-9P **38746-96-2P**
38747-11-4P **38795-20-9P** 55506-29-1P 55506-31-5P
55506-33-7P 55506-34-8P 61589-56-8P 61589-57-9P 61589-58-0P
61589-59-1P
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and cyclization of)

IT 38558-87-1P 59522-36-0P 59522-41-7P 59522-46-2P 59522-49-5P
59522-52-0P 59522-56-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methanolysis of)

IT 6273-79-6P 39992-21-7P 55506-38-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with amines)

IT **38747-00-1P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction of, with chlorophenylacetonitrile)

IT **6362-63-6P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction of, with phenylacetonitriles)

IT 38747-12-5P 38747-15-8P **51780-73-5P** 55506-32-6P
55506-35-9P 59522-37-1P 59522-42-8P 59522-47-3P 59522-53-1P
59522-57-5P 59522-60-0P 61589-54-6P 61589-55-7P
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of)

IT 500-98-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with benzoylformic acid)

IT 31603-77-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with cyanophenylpyruvate)

IT 140-53-4 2947-61-7 6775-77-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with oxalate)

IT 611-73-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phenylacetylglycine)

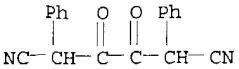
IT 55506-37-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with pulvinc acid lactone)

IT 96-50-4 98-16-8 462-08-8 504-29-0 1072-98-6 5469-69-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with pulvinic acid lactone)

IT **10471-29-1P**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and cyclization of)

RN 10471-29-1 HCAPLUS

CN Hexanedinitrile, 3,4-dioxo-2,5-diphenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



L28 ANSWER 38 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

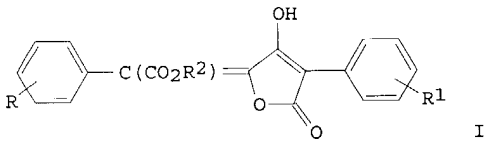
AN 1976:446362 HCAPLUS
DN 85:46362
ED Entered STN: 12 May 1984
TI Ester derivatives of pulvinic acid
IN Sutton, Blaine M.; Walz, Donald T.; Wilson, James W.
PA Smithkline Corp., USA
SO U.S., 7 pp. Division of U.S. 3,826,839.
CODEN: USXXAM
DT **Patent**
LA English
IC C07D
NCL 260343600
CC 27-6 (Heterocyclic Compounds (One Hetero Atom))
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3944571	A	19760316	US 1974-467367	19740506 <--
	US 3826839	A	19740730	US 1971-191051	19711020 <--
	CA 988851	A2	19760511	CA 1974-196994	19740408 <--
PRAI	US 1970-94974		19701203	<--	
	US 1971-191051		19711020	<--	
	CA 1971-127883		19711117	<--	

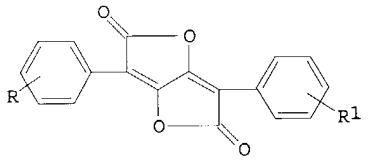
CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3944571	IC	C07D
	NCL	260343600

GI



I



II

AB About 20 pulvinates I (R, R1 = H, p-Cl, m-Cl, p-MeO, p-F, m-MeO, p-EtO, etc.; R2 = Me, Et) were prepared by treating RC6H4CN with Et02CCO2Et and condensation of RC6H4CH(CN)COCO2Et with R1C6H4CN to give RC6H4CH(CN)COCOCH(CN)C6H4R1, which was cyclized and the lactone II hydrolyzed. At 10-50 mg/kg I inhibited adjuvant induced arthritis in rats.
ST pulvinate antiarthritic; inflammation inhibitor pulvinate
IT Arthritis
(inhibitors, pulvinates)
IT Inflammation inhibitors
(pulvinates)
IT 38746-96-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis and cyclization of)
IT 5099-87-6 50886-27-6 59801-33-1 59801-34-2 59801-35-3 59801-36-4 59801-37-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis of)
IT **38747-06-7P** 38747-07-8P
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and cyclization and hydrolysis of)
IT 26548-70-9P 38747-10-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)
IT **10471-29-1P 38747-03-4P 38747-11-4P 38795-20-9P 50689-02-6P**

RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and hydrolysis and cyclization of)

IT 6273-79-6P 20935-72-2P 22628-17-7P 38747-12-5P 38747-15-8P
39992-21-7P 59801-31-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

IT 59801-30-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis or cyclization of)

IT 38746-75-7P 38746-76-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and oxidation of)

IT **6362-63-6P 38747-09-0P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction with phenylacetonitrile)

IT **38747-00-1P 38747-05-6P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction with phenylacetonitriles)

IT 481-59-4P 481-63-0P 481-64-1P 521-52-8P 22628-20-2P 22628-21-3P
27394-71-4P 32883-73-1P 32883-77-5P 37542-20-4P 37542-21-5P
37542-22-6P 37542-24-8P 37542-25-9P 38746-72-4P 38746-73-5P
38746-74-6P 38746-77-9P 38746-78-0P 38746-79-1P 38746-80-4P
38746-81-5P 38746-82-6P 38746-85-9P 38746-86-0P 38746-87-1P
38746-88-2P 38746-89-3P 38746-90-6P 38746-91-7P 38747-14-7P
59801-32-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 93-17-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with cyanophenylpyruvate and with diethyl oxalate)

IT 104-47-2 4439-02-5 19924-43-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with diethyl oxalate)

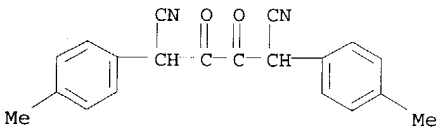
IT 140-29-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ethyl oxalate)

IT 95-92-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phenylacetonitrile)

IT 104-47-2 140-53-4 2947-61-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of,, with ethyl oxalate)

IT **38747-06-7P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and cyclization and hydrolysis of)

RN 38747-06-7 HCAPLUS
CN Hexanedinitrile, 2,5-bis(4-methylphenyl)-3,4-dioxo- (9CI) (CA INDEX NAME)



L28 ANSWER 39 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1976:421417 HCAPLUS
DN 85:21417
ED Entered STN: 12 May 1984
TI Antiarthritic compositions comprising N-heterocyclic pulvinic acid amides
IN Weinstock, Joseph
PA Smithkline Corp., USA
SO U.S., 9 pp. Division of U.S. 3,895,021.
CODEN: USXXAM
DT **Patent**
LA English

IC A61K
NCL 424270000
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 27

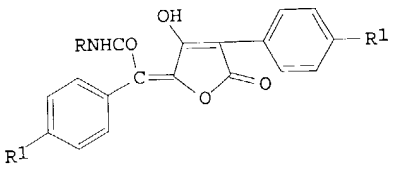
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3947580	A	19760330	US 1975-562628	19750327 <--
	US 3895021	A	19750715	US 1973-393861	19730904 <--
	JP 50058067	A2	19750520	JP 1974-99429	19740828 <--
	JP 58017473	B4	19830407		
	GB 1434156	A	19760505	GB 1974-38260	19740902 <--
	BE 819495	A1	19750303	BE 1974-148174	19740903 <--
PRAI	US 1973-393861		19730904 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3947580	IC	A61K
	NCL	424270000

GI



I

AB Pulvinic acid amides I (R = 2-thiazolyl, 5-chloro-2-thiazolyl, 2-pyridyl, R1 = H; R = 2-thiazolyl, R1 = Cl, EtO), having anti-arthritic activity at 25 mg/kg (rats), were prepared Thus, PhCH2CN condensed with (CO2Et)2 and NaOEt, the PhCH(CN)COCO2Et treated with PhCH2CN in EtOH-NaOEt, the (NCCHPhCO)2 cyclized with AcOH-H2SO4, the pulvinic acid lactonized with Ac2O, and the lactone refluxed with 2-aminothiazole in CHCl3 to give I (R = 2-thiazolyl, R1 = H). Similarly prepared were 4-phenyl-, 4-chloro-4-methyl-, and 4,4'-diacetoxypulvinic acid lactones.

ST antiarthritic heterocyclyl pulvinic amide; diphenyldioxoadiponitrile cyclization; adiponitrile diphenyldioxo cyclization

IT Arthritis
(N-heterocycylpulvinic acid amides as inhibitors of)

IT 140-29-4 140-53-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with ethyl oxalate)

IT 95-92-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with phenylacetonitriles)

IT 38746-96-2 50689-10-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of)

IT **6362-63-6P**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation and condensation with phenylacetonitrile)

IT **10471-29-1P 38747-11-4P 38795-20-9P**
51780-73-5P
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and cyclization of)

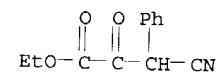
IT 26548-70-9P 38747-01-2P 50689-13-9P 50689-14-0P 55032-45-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and lactonization of)

IT **38747-00-1P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction with (chlorophenyl)acetonitrile)

IT 6273-79-6P 39992-21-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with heterocycyl amines)

IT 38558-83-7P 38747-12-5P 38747-15-8P 51780-75-7P 55506-29-1P
55506-30-4P 55506-31-5P 55506-32-6P 55506-33-7P 55506-34-8P
55506-35-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 55506-38-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with aminothiazole)
IT 31603-77-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ethyl cyanophenylpyruvate)
IT 504-29-0 1072-98-6 5469-69-2 55506-37-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with pulvinic acid lactone)
IT 96-50-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with pulvinic acid lactones)
IT **6362-63-6P**
RL: **SPN (Synthetic preparation)**; **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation and condensation with phenylacetonitrile)
RN 6362-63-6 HCAPLUS
CN Benzenepropanoic acid, .beta.-cyano-.alpha.-oxo-, ethyl ester (9CI) (CA INDEX NAME)



L28 ANSWER 40 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1976:421090 HCAPLUS
DN 85:21090
ED Entered STN: 12 May 1984
TI Tetramic acid analogs of pulvinic acid
IN Weinstock, Joseph
PA Smithkline Corp., USA
SO U.S., 13 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC C07D
NCL 260295500R
CC 27-10 (Heterocyclic Compounds (One Hetero Atom))
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3931207	A	19760106	US 1973-424581	19731214 <--
	US 3984559	A	19761005	US 1975-623226	19751017 <--
PRAI	US 1973-424581		19731214 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3931207	IC	C07D
	NCL	260295500R

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Seven tetramic acid derivs. I (R = thiazolyl, pyridyl, chloropyridyl, 3-F3CC6H4, H, R1 = H; R = thiazolyl, R1 = Cl), inhibitors of adjuvant-induced polyarthritis in rats at 50 mg/kg daily and antibacterials (no data), were prepared (for R .noteq. H) in 7 steps by condensation of 4-R1C6H4CH2CN with (EtO2C)2 via furanone II and tetramic acid lactone III. Ring cleavage of III gave I. To prepare I (R = R1 = H), BzCO2H was condensed with PhCH2CONHCH2CO2H to give anhydride IV which gave I (R = R1 = H) in 3 further steps. Seven further examples were given, but only the various intermediary compds. were characterized.
ST tetramic acid antiarthritic antibacterial; thiazolyltetramic acid pharmaceutical; pyridyltetramic acid pharmaceutical; fluorophenyltetramine acid pharmaceutical; acetonitrile condensation ethyl oxalate; adiponitrile hydrolysis cyclization; pulvinic acid amide cyclization
IT Bactericides, Disinfectants and Antiseptics
Inflammation inhibitors

((carbomethoxyphenylmethylene)phenyltetramic acid derivs.)

IT Lactones
RL: RCT (Reactant); RACT (Reactant or reagent)
(of phenyltetramic acids, cleavage of, with sodium methoxide)

IT Amides, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(of pulvinic acid, cyclization of, tetramic acid lactones by)

IT Nitriles, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(phenylaceto, condensation with diethyl oxalate)

IT 59522-41-7 59522-46-2 59522-49-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(cleavage of, with sodium methoxide)

IT 140-29-4 140-53-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with diethyl oxalate)

IT 95-92-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation with phenylacetonitriles)

IT 59522-51-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of)

IT 50689-13-9 50689-14-0 55032-45-6 59522-55-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(dehydration of)

IT 38746-96-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis of)

IT 50689-10-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis, dehydration, and acetylation of)

IT 38558-87-1P 59522-36-0P 59522-52-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and cleavage with sodium methoxide)

IT **38747-00-1P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation and condensation with (chlorophenyl)acetonitrile)

IT **6362-63-6P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation and condensation with phenylacetonitrile)

IT 59522-35-9P 59522-40-6P 59522-45-1P 59522-48-4P 59534-90-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)

IT 26548-70-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dehydration of)

IT **10471-29-1P 38747-11-4P 38795-20-9P**
51780-73-5P
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and hydrolysis of)

IT 59522-59-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and lactonization of)

IT 59522-58-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and rearrangement of)

IT 38558-83-7P 38747-12-5P 38747-15-8P 51780-75-7P 59522-37-1P
59522-39-3P 59522-42-8P 59522-44-0P 59522-47-3P 59522-50-8P
59522-53-1P 59522-54-2P 59522-57-5P 59522-60-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

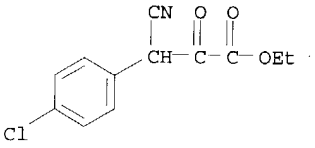
IT 38747-01-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation plus dehydration of)

IT 6362-63-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with (chlorophenyl)acetonitrile)

IT 611-73-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phenylacetylglycine)

IT 98-59-9

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with thiazolylpulvinic acid amide)
IT 39992-21-7 59522-43-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with aminothiazole)
IT 500-98-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with benzoylformic acid)
IT 6273-79-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with heterocyclylamines)
IT 96-50-4 462-08-8 504-29-0 1072-98-6 2646-97-1 5469-69-2
55506-37-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with pulvinic acid lactones)
IT 59522-56-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(ring cleavage of)
IT **38747-00-1P**
RL: **SPN (Synthetic preparation); SPN (Synthetic preparation); PREP (Preparation)**
(preparation and condensation with (chlorophenyl)acetonitrile)
RN 38747-00-1 HCAPLUS
CN Benzenepropanoic acid, 4-chloro-.beta.-cyano-.alpha.-oxo-, ethyl ester (9CI) (CA INDEX NAME)



L28 ANSWER 41 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1975:609414 HCAPLUS
DN 83:209414
ED Entered STN: 12 May 1984
TI Anti-arthritic compositions comprising amide derivatives of pulvinic acid
IN Sutton, Blaine M.; Weinstock, Joseph
PA Smithkline Corp., USA
SO U.S., 5 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC A61K
NCL 424279000
CC 63-6 (Pharmaceuticals)
Section cross-reference(s): 27, 25
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 3907997	A	19750923	US 1971-192588	19711026 <--
PRAI US 1971-192588		19711026 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3907997	IC	A61K
	NCL	424279000

GI For diagram(s), see printed CA Issue.
AB The antiarthritic pulvinic acid amide derivs., I where R1 and R2 = H, C1-4 alkyl, Cl, Br, and F were synthesized and formulations for their administration were described. Thus, 4,4'-dichloropulvinamide [57248-91-6] (whose synthesis was described) 50, Mg stearate 5, and lactose 350 mg/capsule were screened through a Number 40 mesh screen, mixed, and filled into Number 0 hard gelatin capsule.
ST pulvinamide deriv arthritis treatment
IT Arthritis
(pulvinamide derivs. for therapy of)
IT 6273-79-6P
RL: PREP (Preparation)
(prepn, and aminolysis of)
IT 38747-12-5P 39992-21-7P 50688-99-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation and aminolysis of)
IT 31673-63-9P 57216-40-7P 57216-41-8P 57248-91-6P 57248-92-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and antiarthritic activity of)
IT **6362-63-6P 38747-00-1P 38747-05-6P**
57248-93-8P
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP**
(Preparation); RACT (Reactant or reagent)
(preparation and aralkylation of)
IT 26548-70-9P 38747-01-2P 38747-07-8P 50689-13-9P 50689-14-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)
IT **10471-29-1P 38747-06-7P 38747-11-4P**
38795-20-9P
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP**
(Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)
IT 140-29-4 140-53-4 2947-60-6 2947-61-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with diethyl oxalate)
IT 95-92-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phenylacetonitriles)
IT **6362-63-6P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP**
(Preparation); RACT (Reactant or reagent)
(preparation and aralkylation of)
RN 6362-63-6 HCAPLUS
CN Benzenepropanoic acid, .beta.-cyano-.alpha.-oxo-, ethyl ester (9CI) (CA INDEX NAME)

L28 ANSWER 42 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1975:593065 HCAPLUS
DN 83:193065
ED Entered STN: 12 May 1984
TI Antiarthritic phenylvulpinic acid derivatives
IN Sutton, Blaine M.
PA Smithkline Corp., USA
SO U.S., 5 pp. Division of U.S. 3,780,065.
CODEN: USXXAM
DT **Patent**
LA English
IC A61K
NCL 424279000
CC 27-6 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 23, 25
FAN.CNT 2

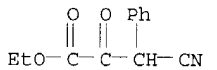
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3896234	A	19750722	US 1973-393235	19730830 <--
	US 3780065	A	19731218	US 1972-279597	19720810 <--
PRAI	US 1971-188555		19711013	<--	
	US 1972-279597		19720810	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3896234	IC	A61K
	NCL	424279000

GI For diagram(s), see printed CA Issue.
AB The title compds. I (R = 3-Ph, 4-Ph, R1 = H; R = H, R1 = 3-Ph, 4-Ph), which inhibited adjuvant arthritis in rats at 20-5 mg/kg, were prepared Thus, condensation of PhCH2CN and (CO2Et)2 gave PhCH(CN)CO2Et, which condensed with PhC6H4CH2Cl to give PhCH(CN)COCOCH(CN)C6H4Ph (II). Hydrolysis and lactonization of II gave the phenylpulvinic acid lactones III, which were hydrolyzed in KOH-MeOH to give I.
ST phenylvulpinate arthritis inhibitor; dioxoadiponitrile hydrolysis cyclization

IT Arthritis
(phenylvulpinates in treatment of)
IT 51780-76-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction of, with ethyl 3-cyano-3-phenylpyruvate)
IT 31603-77-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction with ethyl 3-cyano-3-phenylpyruvate)
IT 140-29-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction with ethyl oxalate)
IT 95-92-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation reaction with phenylacetonitrile)
IT 51780-77-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis of)
IT 51780-88-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and antiarthritic activity of)
IT **6362-63-6P**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation and condensation reaction with biphenylylacetonitriles)
IT **51780-73-5P** 51780-75-7P
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and hydrolysis of)
IT 55506-39-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and lactonization of)
IT **6362-63-6P**
RL: **SPN (Synthetic preparation)**; **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation and condensation reaction with biphenylylacetonitriles)
RN 6362-63-6 HCAPLUS
CN Benzenepropanoic acid, .beta.-cyano-.alpha.-oxo-, ethyl ester (9CI) (CA INDEX NAME)



L28 ANSWER 43 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1975:409762 HCAPLUS
DN 83:9762
ED Entered STN: 12 May 1984
TI .alpha..beta.-Unsaturated esters of vulpinic acid
IN Sutton, Blaine M.
PA Smithkline Corp.
SO U.S., 6 pp. Division of U.S. 3,749,740 (CA 79: 91979w).
CODEN: USXXAM
DT **Patent**
LA English
IC A61K
NCL 424285000
CC 27-6 (Heterocyclic Compounds (One Hetero Atom))
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3865947	A	19750211	US 1973-357982	19730507 <--
	US 3749740	A	19730731	US 1972-276020	19720728 <--
PRAI	US 1971-150209		19710604	<--	
	US 1972-276020		19720728	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3865947	IC	A61K
	NCL	424285000

GI For diagram(s), see printed CA Issue.
AB The vulpinic acid derivs. I (R, R1 = H, 4-MeO; R = R1 = H, 4-Cl, 4-F, 3,4,5-(MeO)C6H3; R2 = H, CH2:CHCO, CH2:CMeCO) were prepared Thus, PhCH2CN was treated with EtO2CCO2Et and the resulting PhCH(CN)COCO2Et treated with

PhCH2CN to give PhCH(CN)COCOCH(CN)Ph which was cyclized to pulvinic acid lactone(II). II and MeOH gave I (R = R1 = H, R2 = H), which with CH2:CHCOCl gave I (R = R1 = H, R2 = COCH:CH2). At 10-150 mg I were antiarthritic.

ST vulpinic acid acryloyl antiarthritic; antiarthritic acryloyl vulpinate; adiponitrile dioxo diphenyl cyclization; cyclization diphenyldioxoadiponitrile; pulvinic acid lactone

IT Arthritis
(vulpinic acid derivative in treatment of)

IT 6273-79-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis of)

IT 521-52-8P 37542-25-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acylation of)

IT **10471-29-1P** 26548-70-9P 38731-08-7P 38747-01-2P **38747-03-4P 38747-06-7P** 38747-07-8P **38795-20-9P 50689-02-6P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and cyclization of)

IT 481-64-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and esterification of)

IT 22628-17-7P 38589-34-3P 39992-21-7P 50886-27-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

IT 38746-87-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with methanol)

IT **38747-00-1P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction with p-chlorophenylacetonitrile)

IT **6362-63-6P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction with phenylacetonitrile)

IT 22628-20-2P 37542-24-8P 38746-88-2P 38746-90-6P 50688-92-1P 50688-93-2P 50688-95-4P 50688-98-7P 50689-05-9P 55697-19-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 104-47-2 140-29-4 140-53-4 459-22-3 2947-61-7 13338-63-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with diethyl oxalate)

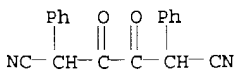
IT 95-92-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phenylacetonitrile)

IT 814-68-6 920-46-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with vulpinic acids)

IT **10471-29-1P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and cyclization of)

RN 10471-29-1 HCAPLUS

CN Hexanedinitrile, 3,4-dioxo-2,5-diphenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



L28 ANSWER 44 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1974:520257 HCAPLUS

DN 81:120257

ED Entered STN: 12 May 1984

TI Substituted 2,5-diphenyl-3,4,6-trihydroxy-.DELTA.2,4-hexadienoic acid lactones (1,4) in the treatment of arthritis

IN Sutton, Blaine M.

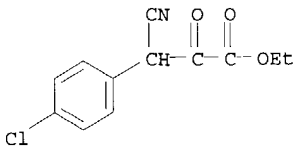
PA Smithkline Corp.
SO U.S., 4 pp. Division of U. S. 3,772,341 (CA 80;133047u).
CODEN: USXXAM
DT **Patent**
LA English
IC A61K
NCL 424279000
CC 25-18 (Noncondensed Aromatic Compounds)
Section cross-reference(s): 63
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 3821398	A	19740628	US 1973-383643	19730730 <--
PRAI US 1970-148890		19700601 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3821398	IC	A61K
	NCL	424279000

GI For diagram(s), see printed CA Issue.
AB Title lactones (I; R = CH2OH, R1 = Ph or substituted phenyl), useful as inhibitors for adjuvant-induced polyarthritis in rats, were prepared by reduction of pulvinic acids I (R = CO2H) (II) with B2H6 in THF. II were prepared in several steps from R1CH2CN. Thus, condensation of PhCH2CN with (CO2Et)2 in THF containing EtONa gave PhCH(CN)COCO2 Et, which with PhCH2CN gave PhCH(CN)COCOCHPhCN. Hydrolysis of the latter with aqueous HOAc-H2SO4 gave II (R1 = Ph).
ST lactone hydroxyphenylhexadienoic acid arthritis; hexadienoic acid hydroxyphenyl lactone; phenylhexadienoic acid hydroxy lactone; pulvinic acid
IT Arthritis
(adjuvant-induced poly-, hydroxyphenyl hexadienoic lactones effect on)
IT 20935-70-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis of)
IT **38747-00-1P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation and condensation with (chlorophenyl)acetonitrile)
IT **38747-09-0P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation and condensation with (dimethoxyphenyl)acetonitrile)
IT **6362-63-6P 41339-41-7P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation and condensation with phenylacetonitrile)
IT **38747-05-6P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation and condensation with tolylacetonitrile)
IT **10471-29-1P 38747-03-4P 38795-20-9P**
RL: RCT (Reactant); **SPN (Synthetic preparation); PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and hydrolysis of)
IT 38747-10-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
IT 26548-70-9P 38747-01-2P 38747-07-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
IT **38747-02-3P 38747-06-7P** 53587-70-5P 53587-71-6P
53658-64-3P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)
IT 93-17-4 104-47-2 140-29-4 140-53-4 1529-41-5 2947-61-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with diethyl oxalate)
IT 95-92-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phenylacetonitrile)
IT **38747-00-1P**
RL: **SPN (Synthetic preparation); PREP (Preparation); PREP (Preparation)**
(preparation and condensation with (chlorophenyl)acetonitrile)
RN 38747-00-1 HCAPLUS
CN Benzenepropanoic acid, 4-chloro-.beta.-cyano-.alpha.-oxo-, ethyl ester (9CI) (CA INDEX NAME)



L28 ANSWER 45 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1974:505256 HCAPLUS
DN 81:105256
ED Entered STN: 12 May 1984
TI 4-Cyclohexylvulpinic acid derivatives in the treatment of arthritis
IN Sutton, Blaine M.
PA Smithkline Corp.
SO U.S., 4 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC A61K
NCL 424279000
CC 27-6 (Heterocyclic Compounds (One Hetero Atom))
FAN.CNT 2

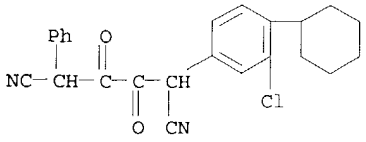
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3821397	A	19740628	US 1973-357762	19730507 <--
	US 3752829	A	19730814	US 1972-282534	19720821 <--
PRAI	US 1971-188439		19711013	<--	
	US 1972-282534		19720821	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3821397	IC	A61K
	NCL	424279000

GI For diagram(s), see printed CA Issue.
AB PhCH2CN was treated with EtO2CCO2Et and the resulting PhCH(CN)COCO2Et treated with 3-chloro-4-cyclohexylphenylacetonitrile and the product cyclized with HOAc to give 3'-chloro-4'-cyclohexylpulvinic acid, which was cyclized and the resulting 3'-chloro-4'-cyclohexylpulvinic acid lactone cleaved with HCl to give the vulpinic oxides I and II. I and II are antiarthritic at 16 mg/kg in rats.
ST vulpinic acid cyclohexyl antiarthritic; antiarthritic cyclohexylvulpinic acid; pulvinic acid chloro cyclohexyl
IT Arthritis
(adjuvant, cyclohexylvulpinic acids as inhibitors for)
IT 50548-55-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and cleavage of)
IT **50548-53-3P** 50548-54-4P
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and cyclization of)
IT **6362-63-6P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction with 3-chloro-4-cyclohexylphenylacetonitrile)
IT 50513-91-2P 50548-56-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 26961-79-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ethyl 3-cyano-3-phenylpyruvate)
IT 140-29-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ethyl oxalate)
IT 95-92-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phenylacetonitrile)
IT **50548-53-3P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and cyclization of)
RN 50548-53-3 HCAPLUS

CN Hexanedinitrile, 2-(3-chloro-4-cyclohexylphenyl)-3,4-dioxo-5-phenyl- (9CI) (CA INDEX NAME)



L28 ANSWER 46 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1974:491367 HCAPLUS
DN 81:91367
ED Entered STN: 12 May 1984
TI Pyridyl ketipate lactones and derivatives in treating arthritis
IN Sutton, Blaine M.
PA Smithkline Corp.
SO U.S., 4 pp. Divison of U.S. 3,714,1733 (CA 78;111148j).
CODEN: USXXAM
DT **Patent**
LA English
IC A61K
NCL 424266000
CC 27-17 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 28
FAN.CNT 4

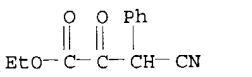
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3818092	A	19740618	US 1972-287381	19720908 <--
	US 3714173	A	19730130	US 1971-160190	19710706 <--
PRAI	US 1971-160190		19710706 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3818092	IC	A61K
	NCL	424266000

GI For diagram(s), see printed CA Issue.
AB PhCH2CN was treated with EtO2CCO2Et and the resulting Ph-CH(CN)COCO2Et treated with 3-pyridylacetonitrile to give 2-phenyl-5-(3-pyridyl)-3,4-dioxoadiponitrile, which was cyclized with H2SO4 and the resulting ketipic acid dilactone I treated with Ac2O to give the ketipate lactone II (R = R1 = H). II (R = H, R1 = Cl, F3C) were similarly prepared II (R = R1 = H) and acyl chlorides gave II (R = H2C:CHCO, H2C:CMeCO, PhCH:CH-CO; R1 = H). At 25 mg/kg II inhibited adjuvant arthritis in rats.
ST ketipate lactone pyridyl antiarthritic; antiarthritic pyridylketipate lactone; cyclization pyridyldioxoadiponitrile; adiponitrile dioxo pyridyl cyclization
IT Arthritis
(adjuvant, inhibition by pyridylketipate lactones)
IT **6362-63-6P 38747-00-1P 40517-14-4P**
40517-16-6P 40517-17-7P 40517-18-8P 40517-19-9P 40517-22-4P
40517-23-5P **40575-04-0P 53353-07-4P** 53353-09-6P
53353-10-9P 53353-56-3P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)
IT 140-53-4 2338-75-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with diethyl oxalate)
IT 6443-85-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ethyl 3-cyano-3-phenylpyruvate)
IT 140-29-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ethyl oxalate)
IT 102-92-1 814-68-6 920-46-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methyl 2-phenyl-5-(3-pyridyl)ketipate lactone)
IT 95-92-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phenylacetonitriles)
IT **6362-63-6P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)

RN 6362-63-6 HCAPLUS
CN Benzenepropanoic acid, .beta.-cyano-.alpha.-oxo-, ethyl ester (9CI) (CA INDEX NAME)



L28 ANSWER 47 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1974:491365 HCAPLUS
DN 81:91365
ED Entered STN: 12 May 1984
TI Pyridyl ketipate lactones and derivatives
IN Sutton, Blaine M.
PA Smithkline Corp.
SO U.S., 3 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC C07D
NCL 260295000R
CC 27-11 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 28

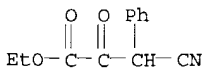
FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3816440	A	19740611	US 1973-393234	19730830 <--
	US 3714173	A	19730130	US 1971-160190	19710706 <--
	US 3781295	A	19731225	US 1972-287189	19720907 <--
PRAI	US 1971-160190		19710706	<--	
	US 1972-287189		19720907	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3816440	IC	C07D
	NCL	260295000R

GI For diagram(s), see printed CA Issue.
AB Ph-CH2CN was treated with EtO2CCO2Et and the resulting PhCH-(CN)COCO2Et treated with 3-pyridylacetonitrile to give 2-phenyl-5-(3-pyridyl)-3,4-dioxoadiponitrile, which was cyclized with AcOH and H2SO4 and the resulting ketipic acid dilactone I treated with Ac2O to give the ketipate lactone II (R = R1 = H). II (R = H, R1 = Cl, CF3) were similarly prepared II (R = R1 = H) and acyl chlorides gave II (R = H2C:CHCO, H2C:CMeCO, PhCH:CHCO; R1 = H). At 25 mg/kg II inhibited adjuvant arthritis in rats.
ST ketipate lactone pyridyl antiarthritic; antiarthritic pyridylketipate lactone; cyclization pyridyldioxoadiponitrile; adiponitrile dioxo pyridyl cyclization
IT Arthritis
(pyridylketipate lactones in treatment of)
IT **6362-63-6P 38747-00-1P 40517-14-4P**
40517-16-6P 40517-17-7P 40517-18-8P 40517-19-9P 40517-22-4P
40517-23-5P **40575-04-0P 53353-07-4P** 53353-08-5P
53353-09-6P 53353-10-9P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)
IT 102-92-1 814-68-6 920-46-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with 2-phenyl-5-(3-pyridyl)ketipate lactone)
IT 140-29-4 140-53-4 2338-75-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with diethyl oxalate)
IT 6443-85-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ethyl 3-cyano-3-phenylpyruvate)
IT 95-92-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phenylacetonitriles)
IT **6362-63-6P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)
RN 6362-63-6 HCAPLUS
CN Benzenepropanoic acid, .beta.-cyano-.alpha.-oxo-, ethyl ester (9CI) (CA INDEX NAME)



L28 ANSWER 48 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1974:133047 HCAPLUS
DN 80:133047
ED Entered STN: 12 May 1984
TI Substituted 2,5-diphenyl-3,4,6-trihydroxy-.DELTA.2,4-hexadienoic acid lactones (1,4)
IN Sutton, Blaine M.
PA Smith Kline French Laboratories
SO U.S., 3 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC C07D
NCL 260343600
CC 25-17 (Noncondensed Aromatic Compounds)
Section cross-reference(s): 27
FAN.CNT 1

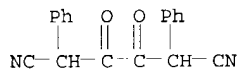
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 3772341	A	19731113	US 1971-148890	19710601 <--
PRAI US 1971-148890		19710601 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3772341	IC	C07D
	NCL	260343600

GI For diagram(s), see printed CA Issue.
AB The title compds. (I; R,R1 = H, Me MeO, CF3, halo) having antiarthritic activity at 25 mg/kg-day in rats were prepared by diborane reduction of pulvinic acid derivs. Thus, a mixture of PhCH2CN and Et oxalate was refluxed in NaOEt solution to give PhCH(CN)COCO2Et, which was refluxed with PhCH2CN in NaOEt solution to give 2,5-diphenyl-3,4-dioxoadiponitrile (II). A mixture of II in H2O, HOAc, and concentrated H2SO4 was refluxed 1 hr to give pulvinic acid, which was reduced with B2H6 in THF to give the lactone (I; R = R1 = H). Similarly prepared were 7 I including a trimethoxyphenyl derivative
ST antiarthritic diaryltrihydroxyhexadienoic lactone; furanone hydroxy diphenyl antiarthritic
IT Arthritis
(diaryltrihydroxyhexadienoic lactones in treatment of)
IT **10471-29-1P 20935-70-0P 38747-03-4P**
38747-06-7P 38795-20-9P 50689-02-6P
52387-78-7P
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and hydrolysis of)
IT **38747-00-1P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction with (chlorophenyl)acetonitrile)
IT **38747-09-0P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction with (dimethoxyphenyl)acetonitrile)
IT **50689-01-5P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction with (fluorophenyl)acetonitrile)
IT **41339-41-7P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction with (methoxyphenyl)acetonitrile)
IT **52387-79-8P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction with (methylphenyl)acetonitrile)
IT **6362-63-6P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)

(preparation and reaction with phenylacetonitrile)
IT 26548-70-9P 38747-01-2P 38747-07-8P 38747-10-3P 50688-96-5P
50688-97-6P 50689-03-7P 50689-07-1P 50689-08-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
IT 93-17-4 104-47-2 140-29-4 140-53-4 459-22-3 2947-61-7
13338-63-1
RL: PROC (Process)
(substitution of, with Et oxalate)
IT **10471-29-1P**
RL: RCT (Reactant); **SPN (Synthetic preparation)**; **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and hydrolysis of)
RN 10471-29-1 HCAPLUS
CN Hexanedinitrile, 3,4-dioxo-2,5-diphenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



L28 ANSWER 49 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1974:95710 HCAPLUS
DN 80:95710
ED Entered STN: 12 May 1984
TI Thiolpulvinic acid derivatives
IN Weinstock, Joseph
PA Smithkline Corp.
SO U.S., 4 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC C07C
NCL 260343600
CC 27-6 (Heterocyclic Compounds (One Hetero Atom))
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3780064	A	19731218	US 1972-267762	19720630 <--
	US 3852462	A	19741203	US 1973-393236	19730830 <--
PRAI	US 1972-267762		19720630 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3780064	IC	C07C
	NCL	260343600

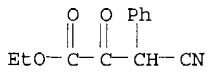
GI For diagram(s), see printed CA Issue.
AB The thiopulvinic acids I (R = Me, Ph, PhCH2, R1 = R2 = H; R = Me, R1 = R2 = Cl; R = Me, R1 = Ph, R2 = H) were prepared Thus, PhCH2CN was treated with EtO2CCO2Et and the resulting PhCH(CN)COCO2Et treated with PhCH2CN to give PhCH(CN)COCOCH(CN)Ph, which was treated with HOAc and the resulting pulvinic acid cyclized to give pulvinic acid lactone. The lactone and MeSH gave I (R = Me, R1 = R2 = H). At 25 mg/kg I inhibited adjuvant arthritis in rats induced by Mycobacterium butyricum.
ST pulvinic acid thio antiarthritic; antiarthritic thiopulvinic acid
IT Arthritis
(thiopulvinic acids in treatment of)
IT 6273-79-6P **6362-63-6P 10471-29-1P** 26548-70-9P
38747-00-1P 38795-20-9P 39992-21-7P
51780-73-5P 51780-75-7P 51780-78-0P 51796-34-0P
51796-35-1P 51796-36-2P 51796-37-3P 51796-38-4P
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of)
IT 31603-77-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with Et cyanophenylpyruvate)
IT 140-29-4 140-53-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with Et oxalate)
IT 95-92-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phenylacetonitrile)
IT 74-93-1 100-53-8 108-98-5

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with pulvinic acid lactone)

IT **6362-63-6P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)

RN 6362-63-6 HCAPLUS

CN Benzenepropanoic acid, .beta.-cyano-.alpha.-oxo-, ethyl ester (9CI) (CA INDEX NAME)



L28 ANSWER 50 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1974:82677 HCAPLUS
DN 80:82677
ED Entered STN: 12 May 1984
TI Pyridyl ketipate lactones and derivatives
IN Sutton, Blaine M.
PA Smithkline Corp.
SO U.S., 3 pp. Division of U.S. 3,714,173 (CA 78;111148j).
CODEN: USXXAM
DT **Patent**
LA English
IC C07D
NCL 260295000R
CC 27-17 (Heterocyclic Compounds (One Hetero Atom))
FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3781295	A	19731225	US 1972-287189	19720907 <--
	US 3714173	A	19730130	US 1971-160190	19710706 <--
	US 3816440	A	19740611	US 1973-393234	19730830 <--
PRAI	US 1971-160190		19710706	<--	
	US 1972-287189		19720907	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3781295	IC	C07D
	NCL	260295000R

GI For diagram(s), see printed CA Issue.

AB The pyridyl ketipate lactones I (R = H, CH2:CHCO, CH2:CMeCO, PhCH:CHCO; R1 = H, Cl; R2 = Me, Et) were prepared Thus, PhCH2CN was treated with the EtO2CCO2Et and NaOEt and the resulting PhCH(CN)COCO2Et treated with 3-pyridylacetonitrile to give 2-phenyl-5-(3-pyridyl)-3,4-dioxoadiponitrile which was treated with concentrated H2SO4 to give I (R = R1 = R2 = H). The acid was esterfied and then acylated with CH2:CHCOCl to give I (R = CH2:CHCO, R1 = H, R2 = Me). At 25 mg/kg I inhibited adjuvant arthritis produced by Mycobacterium butyricum in rats.

ST ketipate lactone pyridyl antiarthritic; antiarthritic pyridyl ketipate lactone; analgesic pyridyl ketipate lactone; antipyretic pyridyl ketipate lactone

IT Arthritis
(inhibitors of, pyridylketipate lactones)

IT Analgesics
Antipyretics
(pyridylketipate lactones)

IT 75-05-8, reactions 140-53-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with Et oxalate)

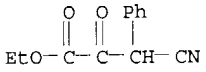
IT 95-92-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with phenylacetonitriles)

IT **6362-63-6P 38747-00-1P 40517-14-4P**
40517-15-5P 40517-16-6P 40517-17-7P 40517-18-8P 40517-19-9P
40517-21-3P 40517-22-4P 40517-23-5P **40575-04-0P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)

IT 6443-85-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with Et 3-cyano-3-phenylpyruvate)

IT 814-68-6
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with Me 2-phenyl-5-(3-pyridyl) ketipate lactone)
IT 102-92-1 920-46-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with Me 2-phenyl-5-(3-pyridyl)ketipate lactone)
IT **6362-63-6P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)
RN 6362-63-6 HCAPLUS
CN Benzenepropanoic acid, .beta.-cyano-.alpha.-oxo-, ethyl ester (9CI) (CA INDEX NAME)



L28 ANSWER 51 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1974:82624 HCAPLUS
DN 80:82624
ED Entered STN: 12 May 1984
TI Phenylvulpinic acid derivatives
IN Sutton, Blaine M.
PA Smithkline Corp.
SO U.S., 4 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC C07D
NCL 260343600
CC 27-6 (Heterocyclic Compounds (One Hetero Atom))
FAN.CNT 2

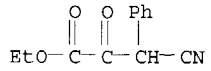
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3780065	A	19731218	US 1972-279597	19720810 <--
	US 3896234	A	19750722	US 1973-393235	19730830 <--
PRAI	US 1971-188555		19711013 <--		
	US 1972-279597		19720810 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3780065	IC	C07D
	NCL	260343600

GI For diagram(s), see printed CA Issue.
AB Antiinflammatory 4-phenylvulpinic acid (I, R = H) was prepared by treating PhCH2CN with (CO2Et)2 and treating the PhCH(CN)COCO2Et with p-PhC6H4CH2CN to give PhCH(CN)COCOCH(CN)C6H4Ph-p. Acid cyclization yielded 4'-phenylpulvinic acid and then its lactone, which was cleaved with base and esterified with MeOH to give I (R = H). Treatment of I (R = H) with acid chlorides gave I (R = CH2:CHCO, CH2:CMeCO, Me2C:CHCO, MeCH:CHCO, PhCH:CHCO). 3-Phenylvulpinic acid was similarly prepared
ST antiinflammatory phenylvulpinic acid; vulpinic acid phenyl antiinflammatory
IT Inflammation inhibitors
(phenylvulpinic acids)
IT **6362-63-6P** 51780-16-6P 51780-17-7P 51780-18-8P 51780-19-9P 51780-20-2P 51780-22-4P **51780-73-5P** 51780-74-6P 51780-75-7P 51780-77-9P 51780-78-0P 51780-79-1P 51780-80-4P 51780-81-5P 51780-82-6P 51780-83-7P 51780-84-8P 51780-86-0P 51780-87-1P 51780-88-2P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)
IT 51780-21-3 51780-85-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with acyl chlorides)
IT 31603-77-7 51780-76-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with cyano(phenyl)pyruvate)
IT 140-29-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with oxalate)
IT 95-92-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phenylacetonitrile)
IT **6362-63-6P**

RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of)
RN 6362-63-6 HCAPLUS
CN Benzenepropanoic acid, .beta.-cyano-.alpha.-oxo-, ethyl ester (9CI) (CA INDEX NAME)



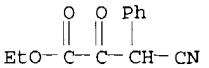
L28 ANSWER 52 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1973:515428 HCAPLUS
DN 79:115428
ED Entered STN: 12 May 1984
TI 4-Cyclohexylvulpinic acid derivatives
IN Sutton, Blaine M.
PA Smith Kline and French Laboratories
SO U.S., 3 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC C07D
NCL 260343600
CC 27-6 (Heterocyclic Compounds (One Hetero Atom))
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3752829	A	19730814	US 1972-282534	19720821 <--
	US 3821397	A	19740628	US 1973-357762	19730507 <--
PRAI	US 1971-188439		19711013	<--	
	US 1972-282534		19720821	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3752829	IC	C07D
	NCL	260343600

GI For diagram(s), see printed CA Issue.
AB PhCH2CN was treated with (CO2Et)2 and the resulting Et 2-cyano-3-phenylpyruvate treated with 3-chloro-4-cyclohexylphenylacetonitrile to give 2-(3-chloro-4-cyclohexylphenyl)-5-phenyl-3,4-dioxoadiponitrile, which with H2O, HOAc, and concentrated H2SO4 gave 3'-chloro-4'-cyclohexylvulpinic acid. The acid was converted to 3'-chloro-4'-cyclohexylvulpinic acid lactone, which with HCl in MeOH gave 3'-chloro-4'-cyclohexylvulpinic acid (I) and 3-chloro-4-cyclohexylvulpinic acid (II). At 16 mg/kg (oral, rat) the Me esters of I and II inhibited development of adjuvant arthritis.
ST vulpinic acid cyclohexyl antiarthritic; antiarthritic chlorocyclohexylvulpinic acid
IT Arthritis
(inhibitor of, cyclohexylvulpinic acids)
IT **6362-63-6P** 50513-91-2P **50548-53-3P** 50548-54-4P 50548-55-5P 50548-56-6P
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of)
IT 26961-79-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ethyl 3-cyano-3-phenylpyruvate)
IT 140-29-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ethyl oxylate)
IT 95-92-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phenylacetonitrile)
IT **6362-63-6P**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of)
RN 6362-63-6 HCAPLUS
CN Benzenepropanoic acid, .beta.-cyano-.alpha.-oxo-, ethyl ester (9CI) (CA INDEX NAME)



L28 ANSWER 53 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1973:491979 HCAPLUS
DN 79:91979
ED Entered STN: 12 May 1984
TI .alpha.,.beta.-Unsaturated esters of vulpinic acid
IN Sutton, Blain M.
PA Smith Kline and French Laboratories
SO U.S., 4 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC C07D
NCL 260343600
CC 27-6 (Heterocyclic Compounds (One Hetero Atom))
FAN.CNT 2

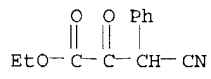
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3749740	A	19730731	US 1972-276020	19720728 <--
	US 3865947	A	19750211	US 1973-357982	19730507 <--
PRAI	US 1971-150209		19710604	<--	
	US 1972-276020		19720728	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3749740	IC	C07D
	NCL	260343600

GI For diagram(s), see printed CA Issue.
AB Vulpinic acid esters (I, R = CH2:CHCO, CH2:CHMeCO, MeCH:CHCO, Me2C:CHCO, PhCH:CHCO; R1, R2 = e.g., H, Cl, MeO, Me), useful for treating arthritis were prepared Thus, PhCH2CN was treated with (CO2Et)2 to give [PhCH(CN)CO]2 which on reaction with Ac2O followed by refluxing in MeOH/HCl gave vulpinic acid. Acylation of this with CH2:CHCOCl gave I (R = CH2:CHCO, R1 = R2 = H).
ST vulpinic acid ester arthritis
IT Arthritis
(vulpinic acid esters in treatment of)
IT 481-64-1P 521-52-8P 6273-79-6P **6362-63-6P**
10471-29-1P 22628-17-7P 22628-20-2P 26548-70-9P
37542-22-6P 37542-23-7P 37542-24-8P 37542-25-9P 38589-34-3P
38731-08-7P 38746-87-1P 38746-88-2P 38746-90-6P **38747-00-1P**
38747-01-2P **38747-03-4P 38747-05-6P**
38747-06-7P 38747-07-8P **38747-11-4P** 38747-12-5P
38795-20-9P 39992-21-7P **41339-41-7P** 50674-92-5P
50688-92-1P 50688-93-2P 50688-94-3P 50688-95-4P 50688-96-5P
50688-97-6P 50688-98-7P 50688-99-8P 50689-00-4P **50689-01-5P**
50689-02-6P 50689-03-7P 50689-04-8P 50689-05-9P
50689-06-0P 50689-07-1P 50689-08-2P 50689-09-3P
50689-10-6P 50689-11-7P 50689-12-8P 50689-13-9P
50689-14-0P 50689-15-1P 50689-16-2P 50886-27-6P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)
IT 104-47-2 140-29-4 140-53-4 459-22-3 2947-61-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with diethyl oxalate)
IT 13338-63-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with ethyl cyanophenylpyruvate)
IT 95-92-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phenylacetonitrile)
IT 102-92-1 814-68-6 920-46-7 10487-71-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with vulpinic acid)
IT **6362-63-6P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)
RN 6362-63-6 HCAPLUS
CN Benzenepropanoic acid, .beta.-cyano-.alpha.-oxo-, ethyl ester (9CI) (CA

INDEX NAME)



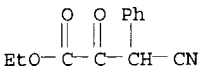
L28 ANSWER 54 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1973:111148 HCAPLUS
DN 78:111148
ED Entered STN: 12 May 1984
TI Pyridyl ketipate lactones and derivatives
IN Sutton, Blaine M.
PA Smith Kline and French Laboratories
SO U.S., 3 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC C07D
NCL 260295000R
CC 27-17 (Heterocyclic Compounds (One Hetero Atom))
FAN.CNT 4

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 3714173	A	19730130	US 1971-160190	19710706 <--
	US 3781295	A	19731225	US 1972-287189	19720907 <--
	US 3818092	A	19740618	US 1972-287381	19720908 <--
	US 3816440	A	19740611	US 1973-393234	19730830 <--
PRAI	US 1971-160190		19710706	<--	
	US 1972-287189		19720907	<--	

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3714173	IC	C07D
	NCL	260295000R

GI For diagram(s), see printed CA Issue.
AB p-RC6H4CH2CN (R = H, Cl) and (CO2Et)2 reacted in EtOH containing NaOEt to give p-RC6H4CH(CN)COCO2Et, which condensed with 3-pyridylacetonitrile (R1CH2CN) in diglyme in the presence of NaH to yield p-RC6H4CH(CN)COCOCHR1CN. The latter compds. were treated with H2SO4 in HOAc give the ketipic acid lactones I (R = H, Cl, R2 = H), which were refluxed in Ac2O and then treated with MeOH containing KOH to give I (R = H, Cl = R2 = Me), which possessed anti-anthritic activity. I (R = H, R2 = Me) was treated with CH2:-CHCOCl, CH2:CMeCOCl, and PhCH:CHCOCl in CHCl3 containing pyridine to yield ketipic lactones II (r = CH2:CHCO, CH2CMeCO, PhCH:CHCO).
ST ketipic acid lactone antiarthritic; pyridine ketipic lactone antiarthritic
IT Arthritis
(Me pyridylketipate lactone effect on)
IT 6443-85-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with cyanopyruvate derivs.)
IT 40517-16-6P 40517-22-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and antiarthritic activity of)
IT **6362-63-6P 38747-00-1P 40517-14-4P**
40517-15-5P 40517-17-7P 40517-18-8P 40517-19-9P 40517-21-3P
40517-23-5P **40575-04-0P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)
IT 140-29-4 140-53-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with diethyl oxalate)
IT 95-92-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with phenylacetonitrile derivs.)
IT **6362-63-6P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)
RN 6362-63-6 HCAPLUS
CN Benzenepropanoic acid, .beta.-cyano-.alpha.-oxo-, ethyl ester (9CI) (CA INDEX NAME)



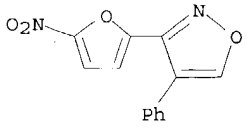
L28 ANSWER 55 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1972:140776 HCAPLUS
DN 76:140776
ED Entered STN: 12 May 1984
TI Antibacterial and antiprotozoal 3-(5-nitro-2-furyl)isoxazoline derivatives
IN Minami, Shinsaku; Matsumoto, Junichi; Shimizu, Masanao; Takase, Yoshiyuki
PA Dainippon Pharmaceutical Co., Ltd.
SO U.S., 10 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC C07D
NCL 260247500R
CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 3631169	A	19711228	US 1966-581192	19660922 <--
PRAI US 1966-581192		19660922 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3631169	IC	C07D
	NCL	260247500R

GI For diagram(s), see printed CA Issue.
AB Is-oxazoles (I, R1 = H, Ac, CN, Me, Et, CO2Et, R2 = H, Me, NH2, Ph, pyridyl, iso-Bu, Et) and isoxazolines (II, R1 = H, Me, R2 = H, Me, CH2Ph, CO2Et, Et, R3 = Et, Ph, H, Me, etc., R4 = H, CH2Cl, CH2CN, CO2Et, etc.; III, R1 = 1-pyrrolidinyl, morpholino, piperidino, NEt2) were prepared by treatment of either 5-nitro-2-furohydroxamoyl halide in the presence of base or of 5-nitrofuronitrile oxide with olefins. Dihydro compds. (II, III) were treated with acid to give I. Thus, treatment of 5-nitro-2-furohydroxamoyl chloride and 1-piperidinocyclohexene with Et3N gave III (R1 = piperidino) (IV). IV at min. inhibitory concentration 0.01-10 .mu.g/ml was active against, e.g., Mycobacterium tuberculosis, Staphylococcus aureus, and Trichomonas vaginalis. About 75 addnl. I, II, and III were prepared similarly. Antimicrobial data for 21 addnl. I, II, and III were given.
ST antibacterial nitrofuryl isoxazoline; antiprotozoal nitrofuryl isoxazoline; furan nitro isoxazolyl antibacterial
IT Bactericides, Disinfectants and Antiseptics
Protozoacides
(nitrofurylisoxazolidines)
IT 7194-20-9P 7194-23-2P 7197-35-5P 7204-88-8P 14730-42-8P
14730-43-9P 14730-45-1P 14730-46-2P **14730-48-4P**
14730-49-5P 14730-50-8P 14730-52-0P 14734-52-2P 14734-55-5P
14734-56-6P 14734-57-7P 14734-58-8P 14734-59-9P 14734-60-2P
14775-77-0P 14775-78-1P 14775-79-2P 14775-81-6P 15154-19-5P
15381-96-1P 15382-00-0P 15427-09-5P 17819-27-1P 17960-17-7P
17960-18-8P 17960-19-9P 17960-21-3P 17960-25-7P 21694-00-8P
21694-05-3P 21706-48-9P 21706-49-0P 21706-51-4P 21706-53-6P
21706-54-7P 21706-56-9P 24247-97-0P 24247-98-1P
24248-00-8P 24970-57-8P 24970-60-3P 24970-61-4P 24970-65-8P
24970-70-5P 24970-72-7P 24970-73-8P 24970-76-1P 24970-78-3P
24974-68-3P 25068-89-7P 26132-60-5P 36241-65-3P 36241-95-9P
36241-98-2P 36241-99-3P 36242-00-9P 36242-01-0P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)
IT **14730-48-4P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)
RN 14730-48-4 HCAPLUS
CN Isoxazole, 3-(5-nitro-2-furanyl)-4-phenyl- (9CI) (CA INDEX NAME)



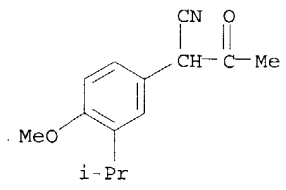
L28 ANSWER 56 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1971:125181 HCAPLUS
DN 74:125181
ED Entered STN: 12 May 1984
TI Hypotensive 3-isopropyltyrosine and 3-isopropyl-.alpha.-alkyltyrosines
IN Hansen, Holger Victor; Meltzer, Robert I.
PA Warner-Lambert Pharmaceutical Co.
SO U.S., 6 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC C07C
NCL 260519000
CC 25 (Noncondensed Aromatic Compounds)
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 3544623	A	19701201	US 1966-550918	19660518 <--
PRAI US 1966-550918		19660518 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3544623	IC	C07C
	NCL	260519000

GI For diagram(s), see printed CA Issue.
AB The title compds. I and II, resp., where R = H or Me, were prepared by 2 procedures: (1) 1-isopropyl-2-alkoxybenzene with Zn(CN)2 in the presence of HCl and AlCl3 gave 3-isopropyl-4-alkoxybenzaldehyde (III). III with hippuric acid in the presence of NaHCO3 suspended in Ac2O gave 4-(3-isopropyl-4-alkoxybenzylidene)-2-phenyloxazol-5-one (IV) which was hydrolyzed with NaOH to 2-benzamido-3-(3-isopropyl-4-alkoxyphenyl)acrylic acid (V) and then hydrogenated (Pd/C) to the propionic acid (VI). VI with HCl gave an alkoxytyrosine which was refluxed with HBr to give I.HBr. In procedure (2), III was reduced by KBH4 to give the benzyl alc. which was converted to the cyanide. Treatment of the cyanide with a lower carboxylic acid alkyl ester in the presence of NaOEt gave the 1-cyanopropanone. After removal of the CN by HCl, it was treated with KCN and (NH4)2CO3 to give the hydantoin (VII). Further treatment with NaOH followed by HBr gave II.HBr. I and II inhibit the action of tyrosine hydroxylase and are useful in the treatment of other ailments resulting from excess amts. of sympathomimetic amines.
ST hypotensive tyrosine isopropyl alkyl
IT 31816-28-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(hypotensive activity)
IT 31816-25-8P 31816-26-9P 31816-27-0P 31816-29-2P **31816-30-5P**
31816-31-6P 31816-32-7P 31816-33-8P 31816-34-9P 31825-29-3P
31825-30-6P 31825-31-7P 31859-25-3P 33537-78-9P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)
IT **31816-30-5P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)
RN 31816-30-5 HCAPLUS
CN Acetoacetonitrile, 2-(4-methoxy-m-cumenyl)- (8CI) (CA INDEX NAME)



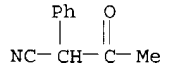
L28 ANSWER 57 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1971:88683 HCAPLUS
DN 74:88683
ED Entered STN: 12 May 1984
TI Light-sensitive diazotype material comprising aryl-substituted acylacetonitriles or their ester or amide derivatives as coupling components
IN Sheehan, John M.
PA Tecnifax Corp.
SO U.S., 5 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC G03C
NCL 096091000
CC 40 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 3558318	A	19710126	US 1968-745697	19680718 <--
PRAI US 1968-745697		19680718 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3558318	IC	G03C
	NCL	096091000

AB The title compns. contain a mixture of a light-sensitive diazonium compound such as 3,4-Me(EtNH)C6H3N2+PF6- (I) and a coupler ArCH(COR) x (II), where R is Me or Ph and X is CN, CO2R1 or CONH2. II (X = CN), prepared from ArCH2CN and RCO2Et in the presence o f Na, are converted to II (X = CO2Et) by the action of dry HCl in EtOH, and into II (X = CONH2) by the action of BF3 in HOAc.
ST diazotype light sensitive compds; light sensitive diazonium compds; diazonium light sensitive compds; nitrile azo coupling components; acetonitriles azo coupling components
IT Diazo process
(couplers for, phenylacetoacetic acid derivs. as)
IT 4433-77-6P **4468-48-8P 5219-07-8P** 5413-05-8P
5415-07-6P 31573-38-3P **63895-78-3P**
RL: **IMF (Industrial manufacture)**; **PREP (Preparation)**
(preparation of)
IT **4468-48-8P**
RL: **IMF (Industrial manufacture)**; **PREP (Preparation)**
(preparation of)
RN 4468-48-8 HCAPLUS
CN Benzeneacetonitrile, .alpha.-acetyl- (9CI) (CA INDEX NAME)



L28 ANSWER 58 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1969:461400 HCAPLUS
DN 71:61400
ED Entered STN: 12 May 1984
TI 3,4-Dihydro-2H-1,3-benzoxazin-2-ones
IN Shavel, John Jr.; Bobowski, George
PA Warner-Lambert Pharmaceutical Co.
SO U.S., 11 pp.
CODEN: USXXAM
DT **Patent**
LA English
IC C07D; A61K
NCL 260244000
CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 3446804	A	19690527	US 1965-504142	19651023 <--
PRAI US 1965-504142		19651023 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3446804	IC	C07DIC A61K
	NCL	260244000

GI For diagram(s), see printed CA Issue.

AB The title compds. (I), useful as antiinflammatory agents, were made by treating 3,4-dihydro-4-hydroxy-2H-1,3-benzoxazin-2-one (prepared according to R. E. Strube, et al., 1964) with R2H. Thus, 6 g. 3,4-dihydro-4-hydroxy-3-methyl-2H-1,3-benzoxazin-2-one and 5.25 g. benzenesulfonamide in 00 ml. C6H6 was refluxed for 2 hrs., while 0.6 ml. H2O was collected in a Dean-Stark trap, to give 9.2 g. 4-phenylsulfonamido-3,4-dihydro-3-methyl-2H-1,3-benzoxazin-2-one, m. 203-4.5.degree. (EtOAc) (decomposition). Similarly prepared were the following (I) (R1, R2, R3, and m.p. given): Me, 4,4-dimethyl-2,6-dioxocyclohexyl, H, 196-7.degree. (decomposition); Me, Ac2CH, H, 136-8.degree.; Me, AcCHCO2Et, H, 140-1.degree.; Me, 2,5-dioxo-1-pyrrolidinyl, H, 182-3.degree.; Me, 5-methyl-2-furyl, H, 130-1.5.degree.; Me, 2-furyl, H, 123-4.degree.; Me, CH2Ac, H, 95-6.5.degree.; Me, CH2COAc, H, 141-3.degree.; Me, CH2COCH2Cl, H, 162-4.degree. (decomposition); Me, AcC(CN)Ph, H, 160-1.degree.; Me, Me, CH2COC6H4Me-p, H, 153-4.degree. (decomposition); Me, 2-thienyl, H, 136-7.degree. (decomposition); Me, C6H4OH-p, H, 219-20.degree.; Me, AcCHBz, H, 163-5.degree. (decomposition); Me, MeNCONHMe, H, 156-7.degree. (decomposition); Me, NHCO2Et, H, 167-8.degree.; Me, NHCO2Et, 6-Cl, 191-2.degree. (decomposition); Me, NHCO2Et, 7-MeNHCO2, 175-8.degree. (decomposition); Me, NHCO2Et, 8-MeO, 166-7.degree.; CH2CH:CH2, NHCO2Et, H, 113-14.degree.; CH2CH:CH2, NHCO2Et, 6-Cl, 156-8.degree. (decomposition); CH2CH:CH2, NHCO2Et, 8-MeO, 127.5-29.degree.; CH2CH:CH2, NHCO2Et, 7-CH2:CHCH2NHCO2, 155.5-7.0.degree.; CH2CH:CH2, NHCO2CH2CH2Cl, 8-MeO, 127-8.degree.; Me, MeNCO2Et, 6-Cl, 96-7.degree.; CH2CH:CH2, MeNCONHMe, H, 148-9.degree.; Me, MeO, 8-MeO, 88-90.degree.; and Me, NHCONH2, H, 203-4.degree. (decomposition).

ST oxazinones dihydro; benzoxazinones; antiinflammatory agents

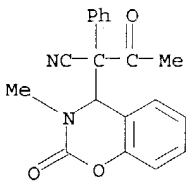
IT Inflammation
(inhibitors of, dihydrobenzoxazinones as)

IT 7646-09-5P 7646-10-8P 7646-11-9P 7646-13-1P 7646-14-2P
7646-15-3P 7646-16-4P 7646-17-5P 7646-18-6P 7646-19-7P
7646-21-1P 7646-22-2P 7646-23-3P 7646-24-4P 7646-25-5P
7646-26-6P 7646-27-7P 7646-28-8P 7678-08-2P 7678-09-3P
7687-92-5P 7687-94-7P 7688-15-5P **23240-88-2P** 23241-00-1P
23241-01-2P 23241-02-3P 23241-03-4P 23241-04-5P 23241-06-7P
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of)

IT **23240-88-2P**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of)

RN 23240-88-2 HCAPLUS

CN 2H-1,3-Benzoxazine-4-acetonitrile, .alpha.-acetyl-3,4-dihydro-3-methyl-2-oxo-.alpha.-phenyl- (8CI) (CA INDEX NAME)



L28 ANSWER 59 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1969:3558 HCAPLUS

DN 70:3558

ED Entered STN: 12 May 1984

TI Ketones and aldehydes

IN Landis, Phillips S.

PA Mobil Oil Corp.

SO U.S., 5 pp.
CODEN: USXXAM

DT **Patent**

LA English

NCL 260094900

CC 25 (Noncondensed Aromatic Compounds)

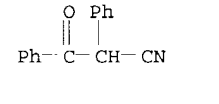
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

PI US 3382226 A 19680507 US 1965-440618 19650317 <--
PRAI US 1965-440618 19650317 <--
CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3382226	NCL	260094900

AB RR1R2CCR3R4COR5 are prepared from RR1R2CH and R3R4C:C(OR6)R5. Thus, a mixture of 1.07 g. .alpha.-methoxystyrene (I) and 8.45 g. PhMe was sealed under N and heated at 250.degree. for 24 hrs. Methane gas was released and the starting material and by-products were distilled The residue was digested with 15 ml. methanol to give .beta.-penylpropiophenone, m. 71-3.degree.. Similarly prepared were: .alpha.-(tetrahydronaphthyl)-acetophenone, b0.05 190-5.degree., 2-(1,2,3,4,5,6-pentamethylbenzyl)-cyclohexan-1-one, m. 121-3.degree., and .beta.-benzoyl-.alpha.-phenylacetonitrile, m. 120-2.degree.. Similar reactions were carried out (reactants and m.p. of products given): hexamethylbenzene and I, 3 products m. 108-28.degree., 115-65.degree., and 124-6.degree.; hexadecane and I, 210-12.degree.; polyethylene (m. 150.degree.) and I, -; hexaethylbenzene, I, -.
ST acetophenones; propiophenones
IT 1083-30-3P **5415-07-6P** 20805-73-6P 26898-23-7P
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)
IT **5415-07-6P**
RL: **SPN (Synthetic preparation); PREP (Preparation)**
(preparation of)
RN 5415-07-6 HCAPLUS
CN Benzenepropanenitrile, .beta.-oxo-.alpha.-phenyl- (9CI) (CA INDEX NAME)



L28 ANSWER 60 OF 60 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1968:96127 HCAPLUS
DN 68:96127
ED Entered STN: 12 May 1984
TI L-.alpha.-Methyl-3,4-dihydroxyphenylalanine, an antihypertensive agent
IN Reinhold, Donald F.; Sletzinger, Meyer
PA Merck and Co., Inc.
SO U.S., 10 pp.
CODEN: USXXAM
DT **Patent**
LA English
NCL 167065000
CC 34 (Synthesis of Amino Acids, Peptides, and Proteins)
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 3344023		19670926	US	19600824 <--

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3344023	NCL	167065000

AB The title compound (L-I) was compared with DL-I and D-I in humans as an antihypertensive. To a solution of 74.3 g. 3,4,5-trimethoxybenzaldehyde in 121 ml. PhMe were added 50.1 g. nitroethane, 3.03 ml. BuNH2, and 3.60 ml. HOAc. The mixture was refluxed, azeotropically removing H2O, and excess reactants removed. Trituration with Skellysolve B gave 1-(2-nitropropen-1-yl)-3,4,5-trimethoxybenzene (II). II (96 g./50 ml. PhMe) was added to 137.4 g. 40-Mesh Fe, 2.75 g. FeCl3.H2O, and 172 ml. H2O. This was refluxed with dropwise addition of 248 ml. HCl, refluxed several more hrs. and cooled. Siliceous filter aid was added, filtered off, and washed with C6H6. The aqueous layer was acidified to pH 2 and extracted with C6H6. The combined C6H6 was extracted with H2O, stirred 1 hr. with 10% NaHSO3, washed with H2O, dried, and evaporated to give 1-(3,4,5-trimethoxyphenyl)-2-propanone (III), an oil. Similarly prepared were 1-(3,4-dimethoxyphenyl)-2-propanone (IV), 1-(3-methoxyphenyl)-2-propanone (V) and 1-(4-hydroxy-3-methoxyphenol)-2-propanone. A solution of 88.5 g. 3,4-dimethoxyphenylacetonitrile in 198 ml. Et propionate was added to 34.5 g. Na in 400 ml. absolute EtOH containing 2% C6H6 and refluxed 4 hrs. Filtration, washing with 200 ml. EtOAc and 200 ml. Et2O, dissoln. in 1200 ml. H2O, cooling to 10.degree., slow addition of 115 ml. HOAc, extraction with Et2O, and drying and concentration of the Et2O yielded 1-cyano-1-(3,4-dimethoxyphenyl)-2-

butanone (VI), an orange oil. VI was slowly added to 250 ml. H_2SO_4 + 60 ml. H_2O at 0-5.degree., heated at 80.degree. for 10 min., at 90.degree. for 3 hrs. and cooled. This was extracted with Et_2O, the extract was washed with 100 ml. 5% $NaHCO_3$ and 100 ml. H_2O, dried, and concentrated to give liquid 1-(3,4-dimethoxyphenyl)-2-butanone. Keeping the temperature at 25-60.degree., 48 g. III in 484 ml. EtOH was added to 165 g. $(NH_4)_2CO_3$ + 35.4 g. KCN in 484 ml. H_2O. Reaction at 55-60.degree. for 18 hrs. and concentration to 1/3 volume in vacuo gave 5-methyl-5-(3,4,5-trimethoxybenzyl)hydantoin (VII), recrystd. from 50% aqueous EtOH. Reaction of 10 g. VII, 45 g. $Ba(OH)_2.8H_2O$, and 226 ml. H_2O in an autoclave at 150.degree., treatment with CO_2 gas at 50.degree., filtration, and washing of the $BaCO_3$ precipitate with hot H_2O, pH adjustment to 6.4 with 2N H_2SO_4 of the combined aqueous portions, hot filtration through siliceous filter aid, and evaporation to dryness gave .alpha.-methyl-.beta.-(3,4,5-trimethoxyphenyl)alanine (VIII). A mixture of 9.15 g. VIII in 124 ml. 48% HBr was refluxed under N for 5 hrs., concentrated in vacuo, flushed with tert-BuOH and H_2O, put on an Amberlite IR-45 hydroxide cycle column, eluted with 800 ml. H_2O, and concentrated to 20 ml. in vacuo to precipitate .alpha.-methyl-.beta.-(3,4,5-trihydroxyphenyl)alanine (IX). Similarly prepared was .alpha.-ethyl-.beta.-(3,4,5-trihydroxyphenyl)alanine; similarly were prepared from IV, .alpha.-methyl-.beta.-(3,4-dihydroxyphenyl)alanine (X), and from V, .alpha.-methyl-.beta.-(3-hydroxyphenyl)alanine. At 10-20.degree. a suspension of 25 g. IX + 250 ml. MeOH was saturated with HCl gas, refluxed for 3 hrs., and allowed to stand 18 hrs. Working under N, repeated in vacuo removal of MeOH and MeOH addition followed by dissoln. in H_2O, and precipitation by NH_4OH addition to pH 8.5 yielded the Me ester of IX. To a mixture of boiled and then cooled 5.73 g. NaOH + 10 ml. H_2O was added 10 g. X and 50 g. ice-H_2O. Addition of 11.13 ml. Ac_2O, reaction at 0.degree. for 1 hr., filtration, washing with of 9:1 iso-PrOH-H_2O, dissoln. in a hot mixture of 100 ml. iso-PrOH + 25 ml. H_2O, filtration, and cooling precipitated .alpha.-methyl-.beta.-(3,4-diacetoxyphenyl)alanine. Reaction of 25 g. X, 100 ml. Ac_2O, and 75 ml. C_5H_5N under N at 90.degree. for 2 hrs., standing overnight at 25.degree., concentration in vacuo, stirring with ice-H_2O, and acidification with 2.5N HCl precipitated N-acetyl-.alpha.-methyl-.beta.-(3,4-diacetoxyphenyl)alanine (XI). Similarly prepared was N-acetyl-.alpha.-methyl-.beta.-(3,4-dimethoxyphenyl)alanine (XII). A slurry of 2.1 g. XII in 4 ml. MeOH and 0.91 g. L-.alpha.-phenylethylamine (L-XIII) in 1 ml. MeOH was prepared, heated to reflux, diluted with 10 ml. MeOH, and refluxed until complete solution occurred. This was filtered through diatomaceous earth, the filter cake washed with 10 ml. H_2O, the MeOH distilled, the solution cooled to 60.degree., seeded with L-XII.L-XIII salt, cooled to 25.degree., aged at 8.degree. for 18 hrs., swirled, and again aged at 80.degree. for 24 hrs. The crude salt was filtered off, washed with cold H_2O, and dried in vacuo at 56.degree., [.alpha.]D 55.degree. (c 1, MeOH). Recrystn. from H_2O gave pure L-N-acetyl-.alpha.-methyl-.beta.-(3,4-dimethoxyphenyl)alanine L-.alpha.-phenyl-ethylamine, [.alpha.]D 69.degree.. A solution of 33.2 g. D-XIII in 50 ml. MeOH was added to slurry of 77 g. XII in 200 ml. MeOH. Addition of 1 l. H_2O, removing the MeOH in vacuo at 50-60.degree., heating to 90.degree., filtration through diatomaceous earth, seeding with D-XII.D-XIII salt, cooling as above, filtration, H_2O washing, and drying over P_2O_5 yielded D-XII.D-XIII salt, [.alpha.]D -59.degree. (c 1, MeOH). The mother liquors + 50 ml. 2.5N NaOH were extracted with $CHCl_3$. Addition of 15 ml. HOAc to the aqueous phase and aging at 8.degree. for 19 hrs. yielded crude L-XII, [.alpha.]D -23.degree.. Treatment with L-XIII and recrystn. from aqueous MeOH gave pure L-XII.L-XIII, [.alpha.]D 68.degree.. Treatment of 25 g. L-XII.L-XIII in 100 ml. H_2O with 27.5 ml. 2.5N NaOH, extraction of the L-XIII with $CHCl_3$, and acidification with HCl yielded L-XII, [.alpha.]D -56.degree.. Treatment of L-XII with 48% HBr (as previously) gave L-X, [.alpha.]D -4 .+-. 2.degree. (c 1, N HCl). The Et ester of L-X had [.alpha.]D -10.degree. (c 1, N HCl). The L-XI quinone salt had [.alpha.]23D -72.5.degree. (c 1, 96% EtOH). Similarly prepared was L-.alpha.-methyl-m-tyrosine, [.alpha.]D -2 .+-. 1.degree. (c 1, 1N HCl). An initial blood pressure of 200 was lowered to 140 with 4.5 g./day DL-I, raised to 200 with 4.5 g./day D-I, and lowered to 130 with 2.25 g./day L-I. Similarly, tests with another subject went from 150 to 110 to 150-160 to 100-110.

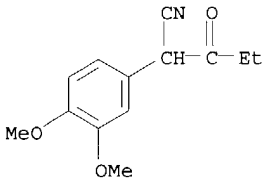
ST ANTIHYPERTENSIVE DIHYDROXY PHENYL; PHENYLALANINES ANTIHYPERTENSIVE; DIHYDROXY; DIHYDROXY PHENYLALANINES; ALANINES

IT Hypertension
(3-(3,4-dihydroxyphenyl)-2-methyl-L-alanine in treatment of)

IT 55-40-3 2799-15-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(as antihypertensive agent)

IT 555-30-6P
RL: PREP (Preparation)
(manufacture of, as antihypertensive agent)

IT 831-74-3P 884-06-0P 976-34-1P 1230-40-6P 5389-29-7P 5556-76-3P
5934-66-7P 6014-30-8P 6892-05-3P 16603-18-2P 16825-27-7P
17762-33-3P 17762-35-5P 17772-80-4P 17772-81-5P
17772-83-7P 17772-88-2P 17772-92-8P
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of)
IT **17762-33-3P**
RL: **SPN (Synthetic preparation)**; **PREP (Preparation)**
(preparation of)
RN 17762-33-3 HCAPLUS
CN Veratronitrile, .alpha.-propionyl- (8CI) (CA INDEX NAME)



=> b home
FILE 'HOME' ENTERED AT 14:42:05 ON 22 SEP 2004

=>

Blank Sheet